



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:17 AM UTC

PDB ID : 4IYO / pdb_00004iyo
Title : Crystal structure of cystathionine gamma lyase from Xanthomonas oryzae pv. oryzae (XometC) in complex with E-site serine, A-site serine, A-site external aldimine structure with aminoacrylate and A-site iminopropionate intermediates
Authors : Ngo, H.P.T.; Kim, J.K.; Kang, L.W.
Deposited on : 2013-01-29
Resolution : 1.80 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](#) ①) 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

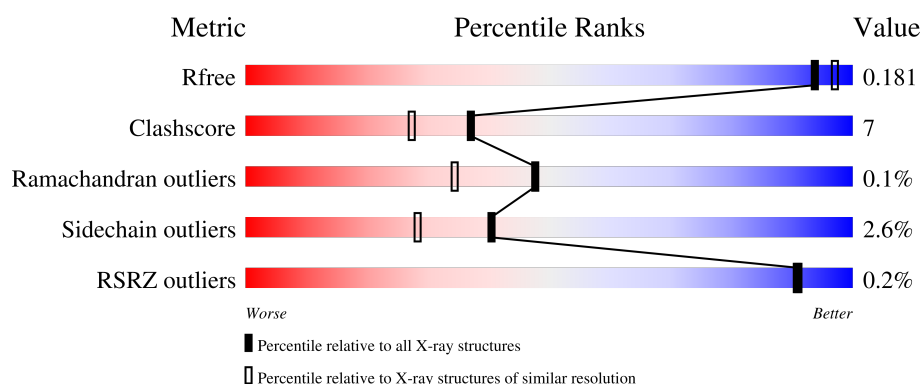
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	397	81% 14% • •
2	B	397	80% 14% • •
2	C	397	82% 11% • •
2	D	397	84% 12% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SER	D	402	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13006 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.

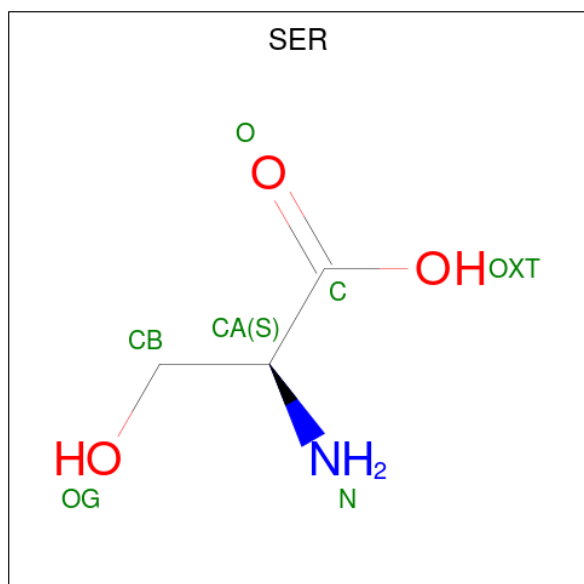
- Molecule 1 is a protein called Cystathionine gamma-lyase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	2881	1825	506	535	15	0	5	0

- Molecule 2 is a protein called Cystathionine gamma-lyase-like protein, LYS201A modified.

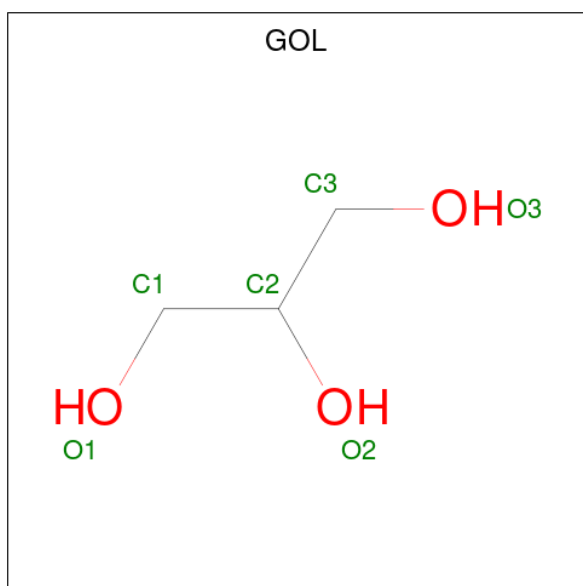
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S		
2	B	381	2890	1828	506	540	1	15	0	4
2	C	381	2890	1828	506	540	1	15	0	4
2	D	384	2924	1846	515	547	1	15	0	5

- Molecule 3 is SERINE (CCD ID: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	3	1	3		
3	B	1	Total	C	N	O	0	0
			7	3	1	3		
3	C	1	Total	C	N	O	0	0
			7	3	1	3		
3	D	1	Total	C	N	O	0	0
			7	3	1	3		
3	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



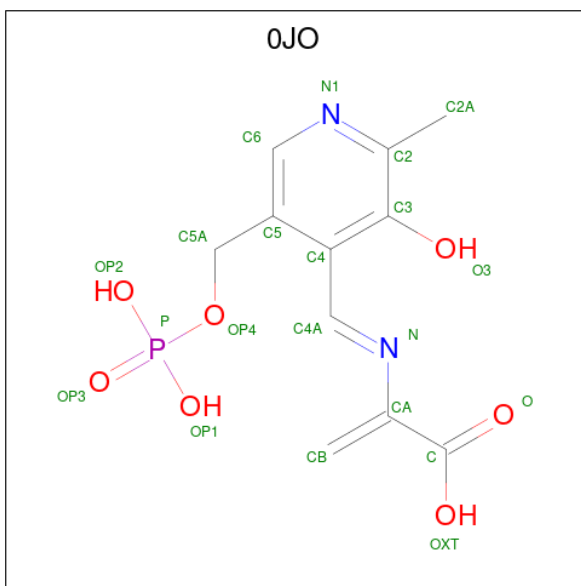
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



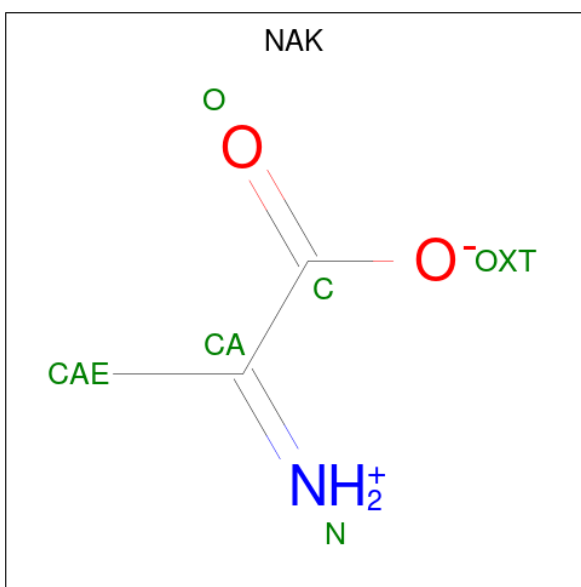
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 2-[(E)-{3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methylidene]amino}prop-2-enoic acid (CCD ID: 0JO) (formula: C₁₁H₁₃N₂O₇P).



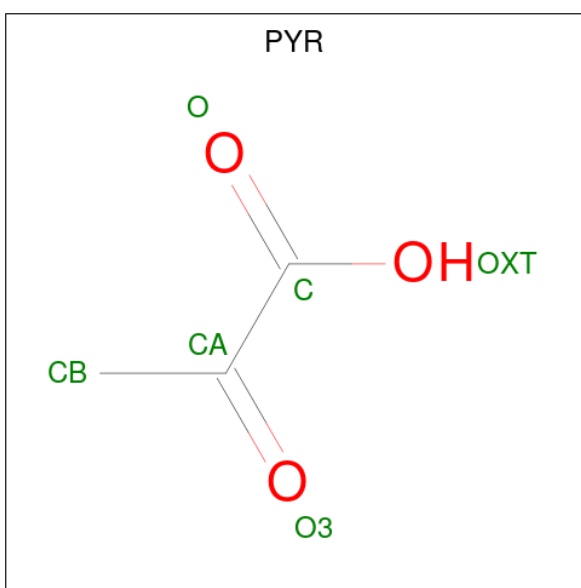
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	
			21	11	2	7	1	

- Molecule 7 is AMINO-ACRYLATE (CCD ID: NAK) (formula: C₃H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			6	3	1	2		
7	C	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 8 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



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

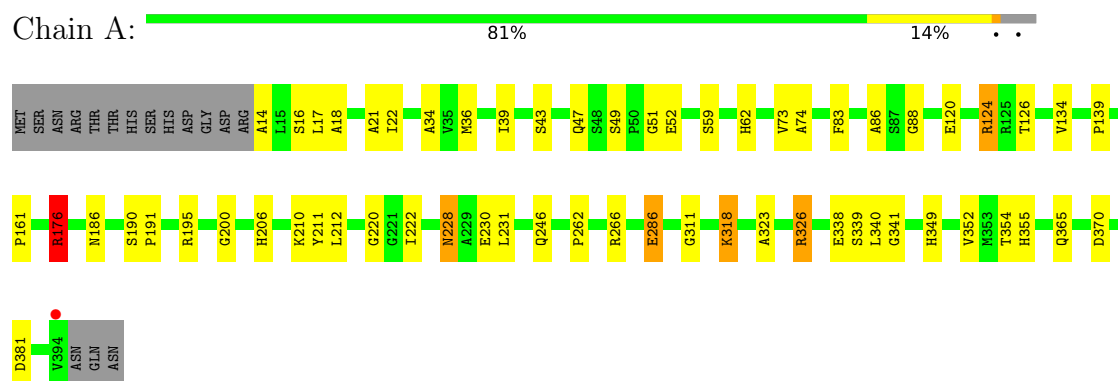
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	324	Total 324	O 324	0	0
9	B	365	Total 365	O 365	0	0
9	C	300	Total 300	O 300	0	0
9	D	335	Total 335	O 335	0	0

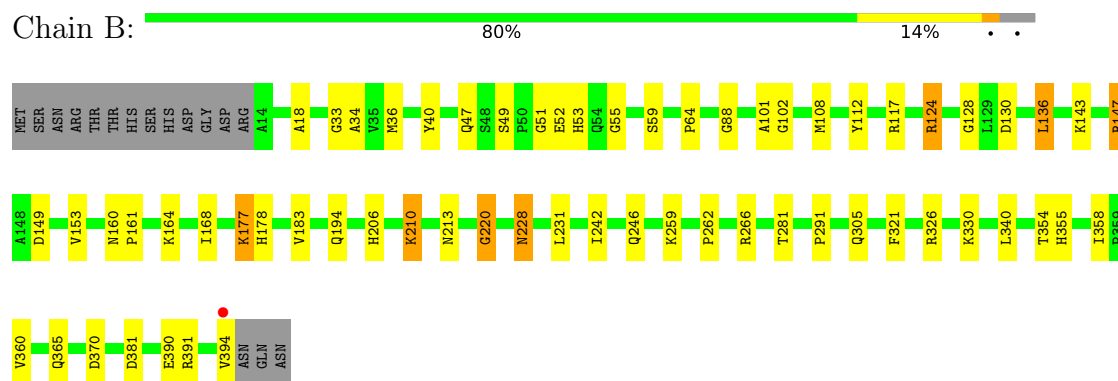
3 Residue-property plots

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.

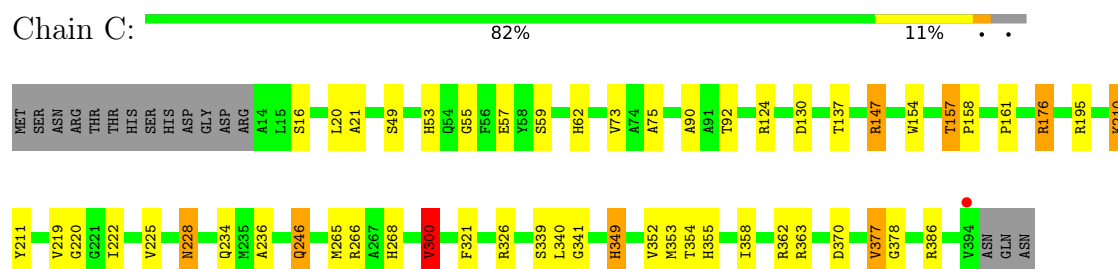
- Molecule 1: Cystathionine gamma-lyase-like protein



- Molecule 2: Cystathionine gamma-lyase-like protein, LYS201A modified



- Molecule 2: Cystathionine gamma-lyase-like protein, LYS201A modified



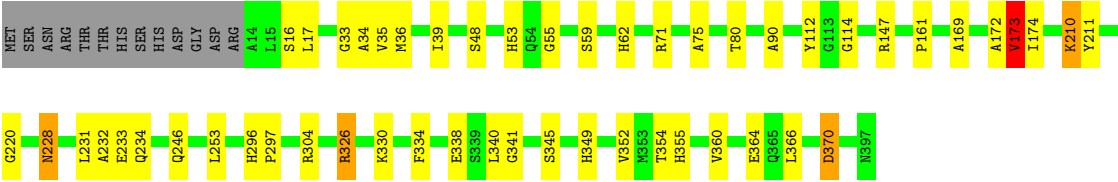
- Molecule 2: Cystathionine gamma-lyase-like protein, LYS201A modified

Chain D:

84%

12%

••



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.32Å 86.34Å 226.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.82 – 1.80 33.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.82-1.80) 100.0 (33.82-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.136 , 0.180 0.137 , 0.181	Depositor DCC
R_{free} test set	6971 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13006	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, SO4, NAK, GOL, LLP, OJO

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	1.53	11/2954 (0.4%)	1.24	7/4007 (0.2%)
2	B	1.56	10/2935 (0.3%)	1.21	6/3982 (0.2%)
2	C	1.57	16/2935 (0.5%)	1.25	7/3982 (0.2%)
2	D	1.51	11/2972 (0.4%)	1.23	4/4031 (0.1%)
All	All	1.54	48/11796 (0.4%)	1.23	24/16002 (0.1%)

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
2	B	0	1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	213	ASN	C-O	7.28	1.32	1.24
1	A	74	ALA	CA-CB	6.64	1.63	1.53
2	D	326	ARG	C-O	-6.58	1.16	1.24
2	D	75	ALA	CA-CB	6.50	1.63	1.53
2	C	75	ALA	CA-CB	6.47	1.63	1.53
1	A	21	ALA	N-CA	6.34	1.54	1.46
2	C	265	MET	N-CA	6.34	1.54	1.46
1	A	311	GLY	N-CA	6.17	1.53	1.45
2	D	360	VAL	CA-CB	6.16	1.61	1.54
2	B	88	GLY	N-CA	6.09	1.53	1.45
2	C	300	VAL	CA-CB	6.06	1.62	1.54
2	C	353	MET	CA-C	6.03	1.55	1.52
2	C	358	ILE	CA-C	6.02	1.57	1.53
2	C	176	ARG	CZ-NH1	5.91	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	ALA	CA-CB	5.87	1.63	1.53
2	D	90	ALA	CA-CB	5.87	1.62	1.53
2	B	183	VAL	N-CA	5.77	1.53	1.46
2	C	358	ILE	N-CA	5.76	1.50	1.46
2	D	172	ALA	CA-CB	5.73	1.62	1.53
2	D	232	ALA	CA-CB	5.71	1.62	1.53
1	A	212	LEU	N-CA	5.70	1.53	1.46
1	A	34	ALA	CA-CB	5.65	1.62	1.53
2	B	281	THR	CA-CB	5.63	1.63	1.53
1	A	22	ILE	CA-CB	5.57	1.61	1.54
2	C	378	GLY	N-CA	5.52	1.51	1.45
2	C	358	ILE	CA-CB	5.51	1.59	1.53
2	B	220	GLY	N-CA	5.51	1.52	1.45
2	B	358	ILE	N-CA	5.50	1.50	1.46
2	D	370	ASP	C-O	-5.50	1.17	1.24
2	B	117	ARG	N-CA	5.48	1.52	1.46
2	B	153	VAL	CA-CB	5.48	1.61	1.54
2	C	21	ALA	N-CA	5.40	1.53	1.46
1	A	86	ALA	CA-CB	5.39	1.62	1.53
2	C	246	GLN	CD-OE1	5.37	1.33	1.23
2	D	174	ILE	C-O	5.35	1.30	1.24
2	D	253	LEU	N-CA	5.27	1.52	1.46
2	B	360	VAL	CA-CB	5.27	1.60	1.54
1	A	134	VAL	CA-CB	5.25	1.62	1.54
2	C	157	THR	CA-CB	5.22	1.61	1.53
1	A	83	PHE	C-O	5.19	1.29	1.23
1	A	286	GLU	N-CA	5.17	1.52	1.46
2	C	225	VAL	N-CA	5.17	1.52	1.46
2	D	80	THR	CB-CG2	5.17	1.69	1.52
1	A	323	ALA	CA-CB	5.15	1.61	1.53
2	C	219	VAL	CA-CB	5.15	1.61	1.54
2	C	236	ALA	C-O	5.11	1.30	1.24
2	D	174	ILE	N-CA	5.07	1.52	1.46
2	C	90	ALA	CA-CB	5.05	1.61	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH1	-7.50	114.00	121.50
2	C	349	HIS	CA-C-N	-7.49	111.25	119.19
2	C	349	HIS	C-N-CA	-7.49	111.25	119.19
2	B	49	SER	N-CA-C	-7.17	101.77	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH2	6.74	125.27	119.20
2	C	300	VAL	N-CA-C	6.30	117.09	110.72
1	A	49	SER	N-CA-C	-6.04	102.78	108.22
2	C	137	THR	N-CA-C	-5.96	105.86	113.01
1	A	126	THR	OG1-CB-CG2	5.82	120.95	109.30
2	C	49	SER	N-CA-C	-5.74	103.06	108.22
2	D	147	ARG	CB-CG-CD	-5.71	98.18	111.30
2	B	112	TYR	CA-C-N	5.46	126.14	120.03
2	B	112	TYR	C-N-CA	5.46	126.14	120.03
1	A	318	LYS	N-CA-C	-5.40	102.29	110.28
2	B	59	SER	N-CA-C	5.39	118.07	111.82
2	D	366	LEU	N-CA-C	-5.31	106.65	113.23
2	D	173	VAL	N-CA-CB	5.27	117.70	110.54
2	C	377	VAL	CA-C-N	-5.26	116.77	122.55
2	C	377	VAL	C-N-CA	-5.26	116.77	122.55
2	B	194	GLN	N-CA-CB	-5.19	101.81	110.99
2	B	242	ILE	N-CA-C	-5.10	105.16	112.35
2	D	48	SER	N-CA-C	-5.06	106.27	112.90
1	A	43	SER	N-CA-C	-5.05	106.29	112.90
1	A	88	GLY	N-CA-C	-5.01	106.72	112.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	206	HIS	Peptide

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	2881	0	2906	47	0
2	B	2890	0	2896	47	0
2	C	2890	0	2897	32	0
2	D	2924	0	2930	38	0
3	A	7	0	4	2	0
3	B	7	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	7	0	4	0	0
3	D	14	0	8	9	0
4	A	6	0	8	0	0
4	C	6	0	8	1	0
4	D	6	0	8	3	0
5	A	5	0	0	0	0
6	A	21	0	9	4	0
7	B	6	0	0	2	0
7	C	6	0	0	2	0
8	B	6	0	0	0	0
9	A	324	0	0	10	0
9	B	365	0	0	7	0
9	C	300	0	0	15	0
9	D	335	0	0	14	0
All	All	13006	0	11682	165	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 7.

All (165) 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:124:ARG:NH1	1:A:124:ARG:HB3	1.30	1.38
1:A:370:ASP:HB2	9:A:775:HOH:O	1.19	1.36
1:A:124:ARG:HH11	1:A:124:ARG:CB	1.38	1.36
2:D:210:LLP:C4'	3:D:402:SER:N	1.96	1.28
2:C:210:LLP:C4'	7:C:402:NAK:N	2.02	1.21
2:B:210:LLP:C4'	7:B:402:NAK:N	2.15	1.09
2:C:210:LLP:H4'1	7:C:402:NAK:N	1.70	1.04
2:D:36:MET:HE1	9:D:812:HOH:O	1.58	1.02
2:D:364:GLU:OE1	9:D:738:HOH:O	1.80	0.98
1:A:36:MET:HE1	9:A:816:HOH:O	1.65	0.97
2:D:210:LLP:H4'1	3:D:402:SER:N	1.78	0.96
2:C:53:HIS:HD2	2:C:55:GLY:H	1.15	0.94
2:B:210:LLP:H4'1	7:B:402:NAK:N	1.83	0.93
2:B:52:GLU:HG3	9:B:730:HOH:O	1.69	0.92
2:D:53:HIS:HD2	2:D:55:GLY:H	1.17	0.91
1:A:210[B]:LYS:HZ1	6:A:404:OJO:C4A	1.84	0.90
1:A:124:ARG:HB3	1:A:124:ARG:HH11	0.74	0.90
2:B:124:ARG:HB2	2:B:124:ARG:HH21	1.37	0.90
2:D:210:LLP:HE3	3:D:402:SER:HA	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:HIS:HD2	2:B:55:GLY:H	1.10	0.89
1:A:52:GLU:HG2	9:A:670:HOH:O	1.72	0.89
2:C:362:ARG:HD3	9:C:526:HOH:O	1.73	0.87
1:A:124:ARG:HH11	1:A:124:ARG:CG	1.87	0.87
2:B:266:ARG:NH1	9:B:847:HOH:O	2.07	0.87
2:B:168:ILE:H	2:B:305:GLN:HE22	1.24	0.86
2:B:143:LYS:HE3	2:B:178:HIS:HE1	1.40	0.84
2:C:386:ARG:HD3	9:C:646:HOH:O	1.77	0.83
2:B:326:ARG:HE	2:B:330:LYS:HD2	1.47	0.80
2:D:220:GLY:HA3	2:D:246:GLN:HE22	1.46	0.80
2:C:124:ARG:HD2	9:C:627:HOH:O	1.79	0.80
4:D:403:GOL:H32	9:D:522:HOH:O	1.81	0.80
1:A:326:ARG:HH11	1:A:326:ARG:HG3	1.47	0.78
2:B:36:MET:HE1	9:D:569:HOH:O	1.83	0.78
1:A:338:GLU:OE1	3:A:401:SER:HB3	1.84	0.77
2:D:210:LLP:CE	3:D:402:SER:HA	2.15	0.77
2:B:147:ARG:NH1	2:B:149:ASP:OD2	2.18	0.77
4:D:403:GOL:H2	9:D:749:HOH:O	1.85	0.76
1:A:124:ARG:NH1	1:A:124:ARG:CB	2.15	0.76
4:C:403:GOL:H12	9:C:568:HOH:O	1.85	0.76
1:A:370:ASP:OD1	9:A:743:HOH:O	2.05	0.74
2:C:220:GLY:HA3	2:C:246:GLN:HE22	1.53	0.73
1:A:220:GLY:HA3	1:A:246:GLN:HE22	1.54	0.72
2:B:124:ARG:HH21	2:B:124:ARG:CB	2.01	0.72
1:A:266:ARG:NH1	9:A:675:HOH:O	2.24	0.71
2:B:220:GLY:HA3	2:B:246:GLN:HE22	1.57	0.70
2:C:363:ARG:NH2	9:C:723:HOH:O	2.24	0.69
2:B:143:LYS:HE3	2:B:178:HIS:CE1	2.26	0.68
2:B:266:ARG:NH2	9:B:829:HOH:O	2.19	0.67
2:B:53:HIS:CD2	2:B:55:GLY:H	2.03	0.67
2:B:124:ARG:NH1	9:B:865:HOH:O	2.27	0.67
2:D:354:THR:OG1	2:D:355:HIS:HD2	1.78	0.66
2:B:259:LYS:HE3	9:D:569:HOH:O	1.94	0.66
1:A:210[B]:LYS:NZ	6:A:404:OJO:C4A	2.58	0.65
1:A:354:THR:OG1	1:A:355:HIS:HD2	1.80	0.63
1:A:36:MET:HE3	9:C:676:HOH:O	1.98	0.63
2:D:210:LLP:C4'	3:D:402:SER:CA	2.77	0.63
2:C:268:HIS:HE1	9:C:560:HOH:O	1.81	0.63
1:A:52:GLU:CG	9:A:670:HOH:O	2.38	0.62
2:B:147:ARG:HH12	2:B:149:ASP:CG	2.08	0.62
1:A:36:MET:CE	9:C:676:HOH:O	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:GLN:HE22	2:B:51:GLY:H	1.48	0.61
1:A:14:ALA:N	9:A:821:HOH:O	2.31	0.61
2:B:354:THR:OG1	2:B:355:HIS:HD2	1.84	0.61
2:B:381:ASP:HB2	2:D:16[A]:SER:OG	2.00	0.61
2:B:326:ARG:HD2	9:B:693:HOH:O	2.01	0.60
2:B:47:GLN:NE2	2:B:51:GLY:H	1.99	0.59
1:A:228:ASN:C	1:A:228:ASN:HD22	2.11	0.59
2:C:228:ASN:C	2:C:228:ASN:HD22	2.10	0.58
2:D:53:HIS:CD2	2:D:55:GLY:H	2.09	0.58
1:A:266:ARG:NH2	9:A:813:HOH:O	2.21	0.58
2:D:71:ARG:HG3	4:D:403:GOL:H31	1.86	0.57
2:C:354:THR:OG1	2:C:355:HIS:HD2	1.87	0.57
2:C:234:GLN:NE2	9:C:734:HOH:O	2.38	0.57
1:A:349:HIS:HD2	1:A:352:VAL:H	1.52	0.57
2:D:210:LLP:H4'1	3:D:402:SER:CA	2.34	0.57
2:D:53:HIS:HD2	2:D:55:GLY:N	1.97	0.57
2:B:391:ARG:O	2:B:394:VAL:HG22	2.05	0.56
2:D:210:LLP:C4	3:D:402:SER:N	2.67	0.56
2:D:228:ASN:HD22	2:D:228:ASN:C	2.14	0.56
2:C:53:HIS:CD2	2:C:55:GLY:H	2.08	0.55
2:C:268:HIS:HD2	2:C:377:VAL:O	1.89	0.55
2:D:364:GLU:HG3	9:D:733:HOH:O	2.06	0.55
2:B:124:ARG:HB2	2:B:124:ARG:NH2	2.16	0.55
1:A:349:HIS:HE1	1:A:370:ASP:O	1.89	0.54
2:C:349:HIS:HE1	2:C:370:ASP:O	1.89	0.54
2:C:362:ARG:NH1	9:C:738:HOH:O	2.39	0.54
9:C:771:HOH:O	2:D:234:GLN:HG2	2.06	0.54
1:A:161:PRO:HD3	1:A:355:HIS:CE1	2.43	0.54
1:A:52:GLU:CD	9:A:670:HOH:O	2.50	0.54
2:B:52:GLU:CG	9:B:730:HOH:O	2.42	0.54
1:A:210[B]:LYS:NZ	6:A:404:OJO:N	2.56	0.53
2:C:386:ARG:CD	9:C:646:HOH:O	2.45	0.53
2:B:147:ARG:NH1	2:B:149:ASP:CG	2.66	0.53
2:B:228:ASN:C	2:B:228:ASN:HD22	2.16	0.52
2:B:228:ASN:ND2	2:B:231:LEU:H	2.07	0.52
2:D:349:HIS:HE1	2:D:370:ASP:O	1.92	0.51
1:A:338:GLU:OE1	3:A:401:SER:CB	2.57	0.51
2:B:108:MET:SD	2:B:136:LEU:HB2	2.49	0.51
1:A:326:ARG:HH11	1:A:326:ARG:CG	2.19	0.51
1:A:210[B]:LYS:HZ1	6:A:404:OJO:CA	2.23	0.50
2:C:57:GLU:CD	9:C:745:HOH:O	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLU:HG3	9:A:594:HOH:O	2.11	0.49
2:C:363:ARG:HD2	9:C:562:HOH:O	2.13	0.49
2:B:53:HIS:HD2	2:B:55:GLY:N	1.93	0.49
1:A:211:TYR:CE1	1:A:341:GLY:HA2	2.48	0.48
2:D:330:LYS:HE2	9:D:789:HOH:O	2.14	0.48
1:A:120:GLU:HA	1:A:124:ARG:HD3	1.95	0.48
2:C:130:ASP:OD2	2:C:147:ARG:NH2	2.47	0.47
2:C:161:PRO:HD3	2:C:355:HIS:CE1	2.49	0.47
2:D:233:GLU:HG2	9:D:635:HOH:O	2.13	0.47
2:D:349:HIS:HD2	2:D:352:VAL:H	1.63	0.47
2:D:304:ARG:NE	9:D:775:HOH:O	2.00	0.46
1:A:18:ALA:HA	1:A:262:PRO:HG2	1.98	0.46
1:A:73:VAL:HG11	1:A:222:ILE:HG21	1.97	0.46
2:B:177:LYS:N	2:B:177:LYS:HD3	2.30	0.46
2:D:169:ALA:O	2:D:173:VAL:HG13	2.15	0.46
2:D:304:ARG:NH2	9:D:775:HOH:O	2.48	0.46
2:B:147:ARG:HH11	2:B:147:ARG:HG3	1.80	0.45
2:D:211:TYR:CE1	2:D:341:GLY:HA2	2.52	0.45
2:B:36:MET:CE	9:D:719:HOH:O	2.64	0.45
1:A:228:ASN:ND2	1:A:231:LEU:H	2.14	0.45
1:A:286:GLU:OE1	1:A:318:LYS:HE3	2.16	0.45
1:A:176:ARG:NH1	1:A:200:GLY:O	2.45	0.45
1:A:39:ILE:HB	2:D:39:ILE:HB	1.99	0.45
1:A:381:ASP:HB2	2:C:16[A]:SER:OG	2.17	0.45
2:B:130:ASP:OD2	2:B:147:ARG:NH2	2.42	0.45
2:C:59[A]:SER:HA	2:C:62:HIS:O	2.16	0.45
1:A:47:GLN:HE22	1:A:51:GLY:H	1.63	0.44
2:B:161:PRO:HD3	2:B:355:HIS:CE1	2.52	0.44
2:C:234:GLN:HB3	9:D:815:HOH:O	2.17	0.44
2:D:35:VAL:O	2:D:36:MET:HE2	2.17	0.44
2:B:33:GLY:O	2:B:34:ALA:C	2.60	0.44
2:D:59:SER:HA	2:D:62:HIS:O	2.17	0.44
2:B:160:ASN:O	2:B:355:HIS:HE1	2.00	0.44
2:C:300:VAL:HG13	9:C:606:HOH:O	2.17	0.43
1:A:47:GLN:NE2	1:A:51:GLY:H	2.17	0.43
2:B:143:LYS:CE	2:B:178:HIS:HE1	2.21	0.43
2:C:211:TYR:CE1	2:C:341:GLY:HA2	2.53	0.43
1:A:59:SER:HA	1:A:62:HIS:O	2.18	0.43
2:C:321:PHE:HB2	2:C:370:ASP:HB3	2.01	0.43
2:C:53:HIS:HD2	2:C:55:GLY:N	1.98	0.42
2:D:326:ARG:NE	2:D:330:LYS:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:OG1	1:A:355:HIS:CD2	2.68	0.42
2:D:161:PRO:HD3	2:D:355:HIS:CE1	2.55	0.42
2:C:157:THR:HA	2:C:158:PRO:C	2.45	0.41
2:C:92:THR:HG23	2:C:154:TRP:CH2	2.56	0.41
2:D:112:TYR:CE2	2:D:114:GLY:HA3	2.55	0.41
1:A:186:ASN:HB3	1:A:206:HIS:CE1	2.56	0.41
2:B:18:ALA:HA	2:B:262:PRO:HG2	2.01	0.41
2:D:228:ASN:ND2	2:D:231:LEU:H	2.19	0.41
1:A:190:SER:HB2	1:A:191:PRO:HD2	2.02	0.41
2:B:102:GLY:HA2	2:B:128:GLY:O	2.21	0.41
2:C:73:VAL:HG11	2:C:222:ILE:HG21	2.03	0.41
2:D:33:GLY:O	2:D:34:ALA:C	2.61	0.41
3:D:401:SER:N	9:D:835:HOH:O	2.54	0.41
2:B:390:GLU:O	2:B:394:VAL:HG13	2.20	0.41
2:D:338:GLU:OE1	3:D:401:SER:HB3	2.20	0.41
2:B:40:TYR:CD1	2:B:64:PRO:HB2	2.56	0.40
2:B:164:LYS:NZ	9:B:845:HOH:O	2.54	0.40
2:B:160:ASN:O	2:B:355:HIS:CE1	2.75	0.40
2:B:321:PHE:HB2	2:B:370:ASP:HB3	2.02	0.40
2:C:349:HIS:HD2	2:C:352:VAL:H	1.70	0.40
2:D:334:PHE:CD2	2:D:345:SER:HB3	2.57	0.40
2:D:296:HIS:HA	2:D:297:PRO:HD3	1.98	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	384/397 (97%)	373 (97%)	10 (3%)	1 (0%)	36	25
2	B	382/397 (96%)	374 (98%)	8 (2%)	0	100	100
2	C	382/397 (96%)	374 (98%)	7 (2%)	1 (0%)	36	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	386/397 (97%)	380 (98%)	6 (2%)	0	100	100
All	All	1534/1588 (97%)	1501 (98%)	31 (2%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	339	SER
1	A	339	SER

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	303/313 (97%)	292 (96%)	11 (4%)	31	18
2	B	301/312 (96%)	293 (97%)	8 (3%)	39	27
2	C	301/312 (96%)	292 (97%)	9 (3%)	36	24
2	D	305/312 (98%)	301 (99%)	4 (1%)	61	54
All	All	1210/1249 (97%)	1178 (97%)	32 (3%)	40	28

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16[A]	SER
1	A	16[B]	SER
1	A	17	LEU
1	A	124	ARG
1	A	139	PRO
1	A	176	ARG
1	A	195	ARG
1	A	228	ASN
1	A	326	ARG
1	A	340	LEU
1	A	365	GLN
2	B	124	ARG

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Mol	Chain	Res	Type
2	B	136	LEU
2	B	147	ARG
2	B	177	LYS
2	B	228	ASN
2	B	291	PRO
2	B	340	LEU
2	B	365	GLN
2	C	20	LEU
2	C	147	ARG
2	C	176	ARG
2	C	195	ARG
2	C	228	ASN
2	C	266	ARG
2	C	300	VAL
2	C	326	ARG
2	C	340	LEU
2	D	17	LEU
2	D	173	VAL
2	D	228	ASN
2	D	340	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	228	ASN
1	A	246	GLN
1	A	271	ASN
1	A	349	HIS
1	A	355	HIS
2	B	47	GLN
2	B	53	HIS
2	B	54	GLN
2	B	178	HIS
2	B	194	GLN
2	B	228	ASN
2	B	240	ASN
2	B	246	GLN
2	B	271	ASN
2	B	305	GLN
2	B	355	HIS
2	B	365	GLN

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Mol	Chain	Res	Type
2	C	53	HIS
2	C	54	GLN
2	C	228	ASN
2	C	234	GLN
2	C	240	ASN
2	C	246	GLN
2	C	268	HIS
2	C	271	ASN
2	C	349	HIS
2	C	355	HIS
2	C	365	GLN
2	D	53	HIS
2	D	54	GLN
2	D	228	ASN
2	D	246	GLN
2	D	271	ASN
2	D	349	HIS
2	D	355	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	LLP	B	210	2	23,24,25	2.63	11 (47%)	25,32,34	2.18	9 (36%)
2	LLP	D	210	2	23,24,25	2.27	8 (34%)	25,32,34	1.99	9 (36%)
2	LLP	C	210	2	23,24,25	2.53	8 (34%)	25,32,34	2.20	7 (28%)

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	LLP	B	210	2	-	4/16/17/19	0/1/1/1
2	LLP	D	210	2	-	7/16/17/19	0/1/1/1
2	LLP	C	210	2	-	6/16/17/19	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	210	LLP	C3-C2	7.33	1.48	1.41
2	C	210	LLP	C3-C2	6.36	1.47	1.41
2	D	210	LLP	C3-C2	5.00	1.46	1.41
2	C	210	LLP	C4-C5	4.92	1.48	1.42
2	B	210	LLP	C4-C5	4.82	1.48	1.42
2	D	210	LLP	C4-C5	4.67	1.48	1.42
2	C	210	LLP	P-OP3	-3.84	1.40	1.54
2	C	210	LLP	P-OP2	-3.83	1.40	1.54
2	B	210	LLP	P-OP3	-3.78	1.40	1.54
2	B	210	LLP	C4-C3	3.75	1.47	1.41
2	D	210	LLP	P-OP3	-3.67	1.41	1.54
2	D	210	LLP	P-OP2	-3.60	1.41	1.54
2	C	210	LLP	OP4-C5'	-3.49	1.32	1.44
2	D	210	LLP	C4-C3	3.36	1.46	1.41
2	B	210	LLP	OP4-C5'	-3.13	1.33	1.44
2	B	210	LLP	P-OP2	-3.06	1.43	1.54
2	D	210	LLP	C4'-NZ	3.05	1.37	1.27
2	C	210	LLP	P-OP1	-3.04	1.41	1.50
2	D	210	LLP	OP4-C5'	-3.00	1.33	1.44
2	B	210	LLP	P-OP1	-2.98	1.41	1.50
2	C	210	LLP	C4-C3	2.96	1.46	1.41
2	B	210	LLP	CD-CE	2.58	1.60	1.51
2	C	210	LLP	C4'-NZ	2.37	1.35	1.27
2	B	210	LLP	C4'-NZ	2.27	1.34	1.27
2	D	210	LLP	P-OP4	-2.19	1.53	1.60
2	B	210	LLP	CB-CA	-2.05	1.50	1.53
2	B	210	LLP	CE-NZ	2.02	1.51	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	LLP	OP4-C5'-C5	6.24	121.05	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	210	LLP	OP4-C5'-C5	5.41	119.50	109.36
2	C	210	LLP	C3-C4-C5	-4.35	114.78	118.28
2	B	210	LLP	OP2-P-OP4	-4.30	95.46	106.67
2	D	210	LLP	CE-NZ-C4'	4.20	132.16	118.72
2	D	210	LLP	C2'-C2-C3	-4.17	115.92	120.80
2	C	210	LLP	CE-NZ-C4'	3.89	131.18	118.72
2	B	210	LLP	CE-NZ-C4'	3.66	130.43	118.72
2	D	210	LLP	C5-C4-C4'	3.31	126.58	121.47
2	C	210	LLP	C2'-C2-N1	3.19	123.66	117.64
2	D	210	LLP	C2'-C2-N1	3.04	123.37	117.64
2	B	210	LLP	OP3-P-OP2	2.96	118.88	107.80
2	C	210	LLP	OP2-P-OP4	-2.77	99.46	106.67
2	D	210	LLP	OP4-C5'-C5	2.70	114.41	109.36
2	C	210	LLP	C4-C3-C2	2.67	121.64	120.14
2	C	210	LLP	C2'-C2-C3	-2.54	117.83	120.80
2	B	210	LLP	C4-C3-C2	-2.53	118.72	120.14
2	D	210	LLP	CD-CE-NZ	2.39	117.16	110.83
2	D	210	LLP	C3-C4-C5	-2.35	116.39	118.28
2	D	210	LLP	OP3-P-OP2	2.25	116.24	107.80
2	B	210	LLP	C4-C4'-NZ	-2.19	113.94	124.04
2	B	210	LLP	C3-C4-C5	-2.19	116.52	118.28
2	D	210	LLP	C4-C3-C2	-2.09	118.97	120.14
2	B	210	LLP	O3-C3-C2	2.08	121.89	117.58
2	B	210	LLP	C6-N1-C2	2.05	122.91	119.20

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	210	LLP	O-C-CA-CB
2	C	210	LLP	O-C-CA-CB
2	D	210	LLP	O-C-CA-CB
2	B	210	LLP	CG-CD-CE-NZ
2	C	210	LLP	CG-CD-CE-NZ
2	D	210	LLP	CG-CD-CE-NZ
2	C	210	LLP	CA-CB-CG-CD
2	D	210	LLP	C3-C4-C4'-NZ
2	D	210	LLP	C5-C4-C4'-NZ
2	D	210	LLP	C-CA-CB-CG
2	B	210	LLP	CD-CE-NZ-C4'
2	D	210	LLP	CD-CE-NZ-C4'
2	B	210	LLP	C3-C4-C4'-NZ

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Mol	Chain	Res	Type	Atoms
2	C	210	LLP	C3-C4-C4'-NZ
2	C	210	LLP	C5-C4-C4'-NZ
2	C	210	LLP	CD-CE-NZ-C4'
2	D	210	LLP	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	210	LLP	2	0
2	D	210	LLP	7	0
2	C	210	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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$
3	SER	B	401	-	4,6,6	1.14	0	2,7,7	1.09	0
3	SER	C	401	-	4,6,6	1.22	1 (25%)	2,7,7	2.57	1 (50%)
4	GOL	A	402	-	5,5,5	0.68	0	5,5,5	0.26	0
4	GOL	C	403	-	5,5,5	0.47	0	5,5,5	1.30	0
8	PYR	B	403	-	5,5,5	2.94	2 (40%)	3,6,6	2.22	2 (66%)
4	GOL	D	403	-	5,5,5	0.42	0	5,5,5	0.87	0
3	SER	D	402	-	4,6,6	1.79	1 (25%)	2,7,7	0.10	0
3	SER	D	401	-	4,6,6	0.88	0	2,7,7	1.67	1 (50%)
6	OJO	A	404	-	20,21,21	2.59	7 (35%)	23,30,30	2.03	7 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAK	B	402	-	4,5,5	1.11	0	4,6,6	3.18	3 (75%)
7	NAK	C	402	-	4,5,5	1.33	1 (25%)	4,6,6	3.82	2 (50%)
5	SO4	A	403	-	4,4,4	0.48	0	6,6,6	0.32	0
3	SER	A	401	-	4,6,6	1.22	1 (25%)	2,7,7	1.59	1 (50%)

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	SER	B	401	-	-	0/6/6/6	-
3	SER	C	401	-	-	0/6/6/6	-
4	GOL	A	402	-	-	0/4/4/4	-
4	GOL	C	403	-	-	2/4/4/4	-
8	PYR	B	403	-	-	0/4/4/4	-
4	GOL	D	403	-	-	4/4/4/4	-
3	SER	D	402	-	-	2/6/6/6	-
3	SER	D	401	-	-	0/6/6/6	-
6	OJO	A	404	-	-	0/11/15/15	0/1/1/1
7	NAK	B	402	-	-	2/2/4/4	-
7	NAK	C	402	-	-	2/2/4/4	-
3	SER	A	401	-	-	1/6/6/6	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	404	OJO	C4-C3	5.94	1.50	1.41
6	A	404	OJO	C3-C2	5.60	1.46	1.41
8	B	403	PYR	O-C	5.03	1.35	1.22
6	A	404	OJO	C4A-N	4.76	1.34	1.28
6	A	404	OJO	C2A-C2	3.76	1.56	1.50
8	B	403	PYR	CA-C	-3.70	1.42	1.54
3	D	402	SER	OXT-C	-3.07	1.20	1.30
6	A	404	OJO	C4-C5	2.78	1.45	1.42
6	A	404	OJO	OXT-C	-2.52	1.23	1.30
7	C	402	NAK	OXT-C	-2.30	1.24	1.30
3	A	401	SER	OXT-C	-2.21	1.23	1.30
6	A	404	OJO	C4-C4A	2.20	1.51	1.46
3	C	401	SER	OXT-C	-2.11	1.23	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	402	NAK	CAE-CA-C	6.60	124.34	118.11
6	A	404	OJO	C3-C4-C5	-5.50	113.86	118.28
7	B	402	NAK	CAE-CA-C	4.69	122.54	118.11
6	A	404	OJO	C4-C3-C2	-3.70	118.06	120.14
7	C	402	NAK	O-C-CA	-3.66	116.87	121.35
7	B	402	NAK	O-C-CA	-3.65	116.89	121.35
3	C	401	SER	OXT-C-O	-3.63	115.85	124.08
8	B	403	PYR	OXT-C-O	-3.05	116.64	123.90
6	A	404	OJO	C4-C4A-N	-2.95	116.21	123.01
6	A	404	OJO	C5-C4-C4A	2.80	125.79	121.47
6	A	404	OJO	C2A-C2-C3	-2.67	117.67	120.80
6	A	404	OJO	C6-C5-C4	2.50	122.52	118.21
3	D	401	SER	OXT-C-O	-2.34	118.76	124.08
7	B	402	NAK	OXT-C-CA	2.14	121.05	116.50
3	A	401	SER	OXT-C-O	-2.13	119.25	124.08
8	B	403	PYR	O3-CA-CB	-2.08	115.10	119.77
6	A	404	OJO	OP4-P-OP3	-2.01	101.01	106.44

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	SER	O-C-CA-CB
3	D	402	SER	N-CA-CB-OG
4	C	403	GOL	C1-C2-C3-O3
4	D	403	GOL	O1-C1-C2-C3
7	B	402	NAK	OXT-C-CA-CAE
7	B	402	NAK	O-C-CA-CAE
7	C	402	NAK	O-C-CA-CAE
4	D	403	GOL	C1-C2-C3-O3
4	D	403	GOL	O1-C1-C2-O2
4	C	403	GOL	O2-C2-C3-O3
3	D	402	SER	C-CA-CB-OG
7	C	402	NAK	OXT-C-CA-CAE
4	D	403	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 23 short contacts:

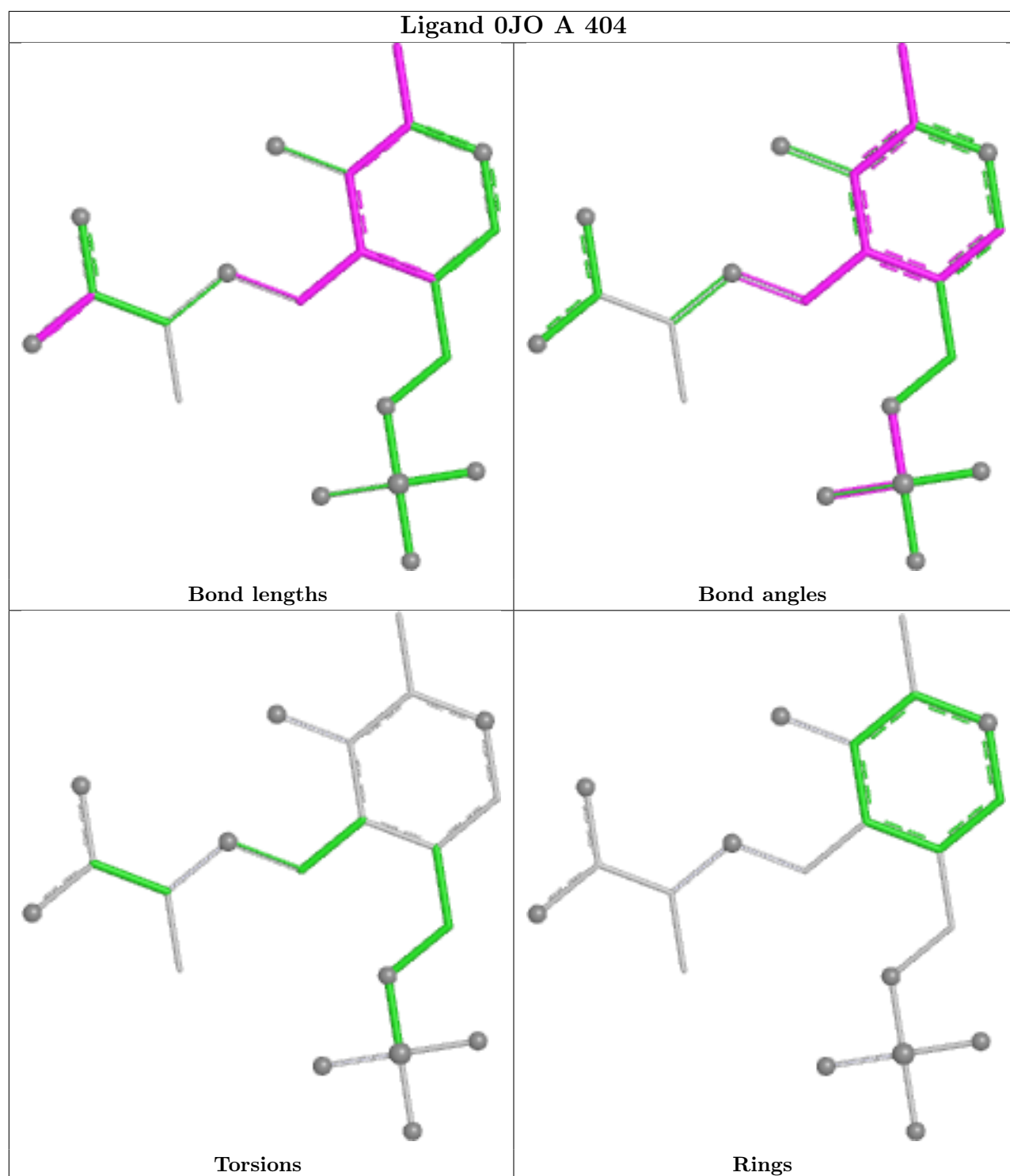
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403	GOL	3	0
3	D	402	SER	7	0
3	D	401	SER	2	0
6	A	404	OJO	4	0
7	B	402	NAK	2	0
7	C	402	NAK	2	0
3	A	401	SER	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	381/397 (95%)	-0.85	1 (0%) 90 90	7, 14, 26, 37	5 (1%)
2	B	380/397 (95%)	-0.86	1 (0%) 90 90	8, 14, 25, 39	4 (1%)
2	C	380/397 (95%)	-0.62	1 (0%) 90 90	8, 17, 34, 49	4 (1%)
2	D	383/397 (96%)	-0.80	0 100 100	7, 15, 26, 55	5 (1%)
All	All	1524/1588 (95%)	-0.78	3 (0%) 91 91	7, 15, 29, 55	18 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	VAL	2.6
2	C	394	VAL	2.4
2	B	394	VAL	2.1

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	LLP	B	210	24/25	0.97	0.07	9,17,24,25	0
2	LLP	C	210	24/25	0.97	0.07	11,17,26,27	0
2	LLP	D	210	24/25	0.97	0.07	10,16,28,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

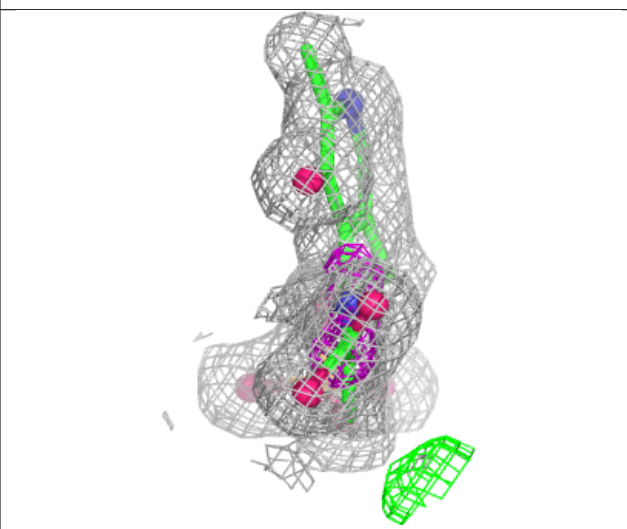
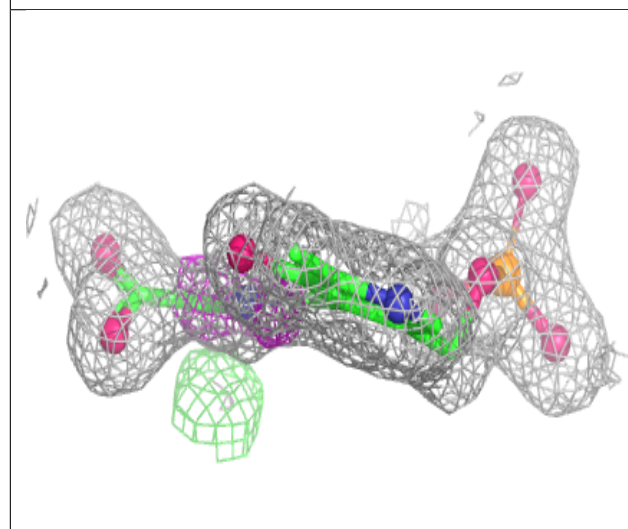
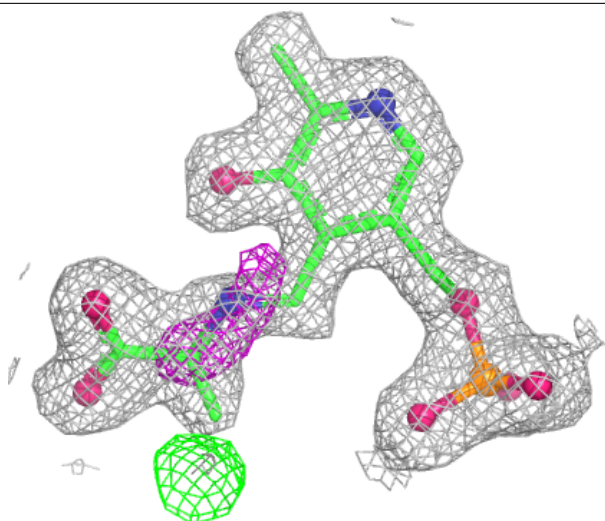
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	C	403	6/6	0.89	0.11	26,34,41,53	0
4	GOL	D	403	6/6	0.92	0.11	17,41,41,44	0
8	PYR	B	403	6/6	0.92	0.10	18,23,30,34	0
7	NAK	C	402	6/6	0.93	0.10	27,33,38,38	0
3	SER	A	401	7/7	0.94	0.07	26,30,30,31	0
3	SER	C	401	7/7	0.95	0.06	30,31,32,33	0
3	SER	D	402	7/7	0.95	0.10	18,21,24,30	0
3	SER	B	401	7/7	0.95	0.06	19,20,23,26	0
3	SER	D	401	7/7	0.96	0.06	21,23,26,27	0
7	NAK	B	402	6/6	0.96	0.07	20,24,31,32	0
4	GOL	A	402	6/6	0.97	0.05	17,18,20,20	0
6	OJO	A	404	21/21	0.98	0.05	11,19,25,26	0
5	SO4	A	403	5/5	0.98	0.11	32,37,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 0JO A 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.