



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:06 PM UTC

PDB ID : 6LD7 / pdb_00006ld7
Title : Native Structure of cystathionine gamma synthase (XometB) from Xanthomonas oryzae pv. oryzae
Authors : Ngo, H.P.T.; Nguyen, T.D.Q.; Kang, L.W.
Deposited on : 2019-11-20
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

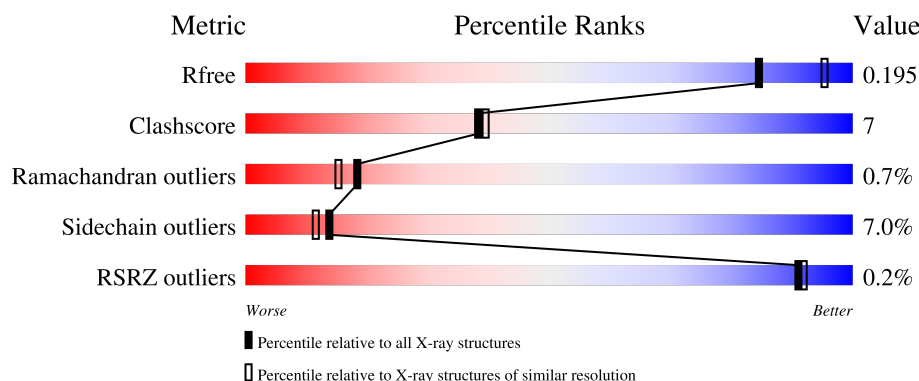
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	408	 77% 14% . . 5%
1	B	408	 73% 16% . . 5%
1	C	408	 74% 16% . . 5%
1	D	408	 75% 14% . . 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12288 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-synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	P	S	0	2	0
			2891	1826	507	550	1	7			
1	B	386	Total	C	N	O	P	S	0	1	0
			2878	1819	506	545	1	7			
1	C	388	Total	C	N	O	P	S	0	1	0
			2892	1826	508	550	1	7			
1	D	386	Total	C	N	O	P	S	0	2	0
			2884	1822	506	548	1	7			

There are 16 discrepancies between the modelled and reference sequences:

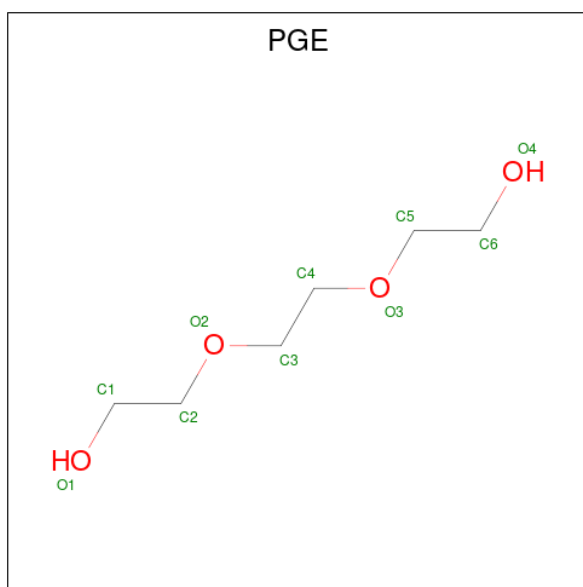
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q5H1U9
A	-1	SER	-	expression tag	UNP Q5H1U9
A	0	HIS	-	expression tag	UNP Q5H1U9
A	134	VAL	ASP	engineered mutation	UNP Q5H1U9
B	-2	GLY	-	expression tag	UNP Q5H1U9
B	-1	SER	-	expression tag	UNP Q5H1U9
B	0	HIS	-	expression tag	UNP Q5H1U9
B	134	VAL	ASP	engineered mutation	UNP Q5H1U9
C	-2	GLY	-	expression tag	UNP Q5H1U9
C	-1	SER	-	expression tag	UNP Q5H1U9
C	0	HIS	-	expression tag	UNP Q5H1U9
C	134	VAL	ASP	engineered mutation	UNP Q5H1U9
D	-2	GLY	-	expression tag	UNP Q5H1U9
D	-1	SER	-	expression tag	UNP Q5H1U9
D	0	HIS	-	expression tag	UNP Q5H1U9
D	134	VAL	ASP	engineered mutation	UNP Q5H1U9

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is water.

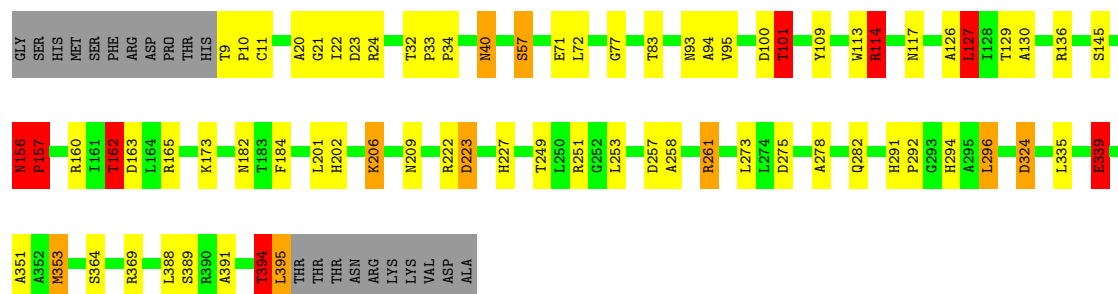
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total	O	0	0
			146	146		
4	B	187	Total	O	0	0
			187	187		
4	C	176	Total	O	0	0
			176	176		
4	D	163	Total	O	0	0
			163	163		

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.

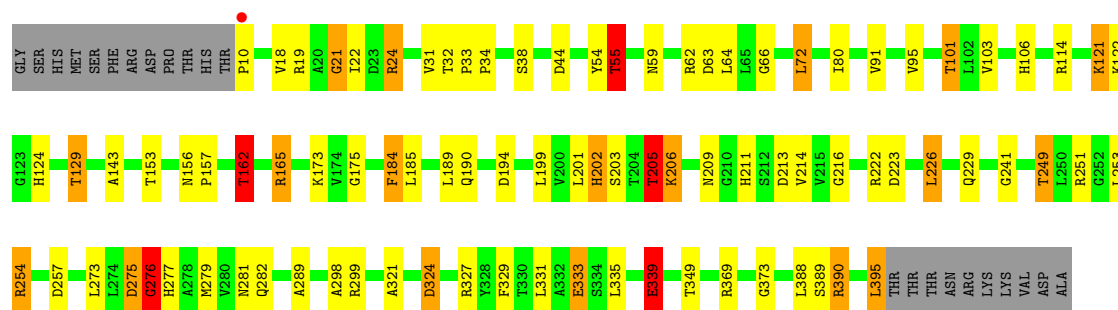
• Molecule 1: Cystathionine gamma-synthase

Chain A: 



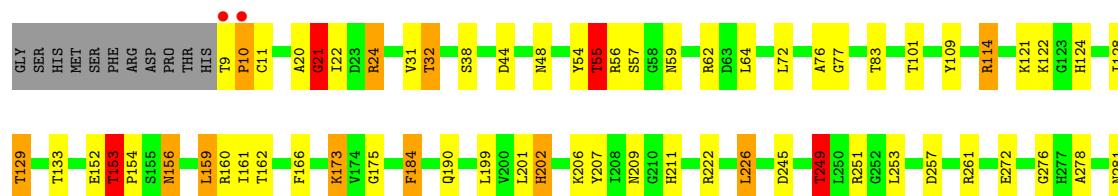
• Molecule 1: Cystathionine gamma-synthase

Chain B: 



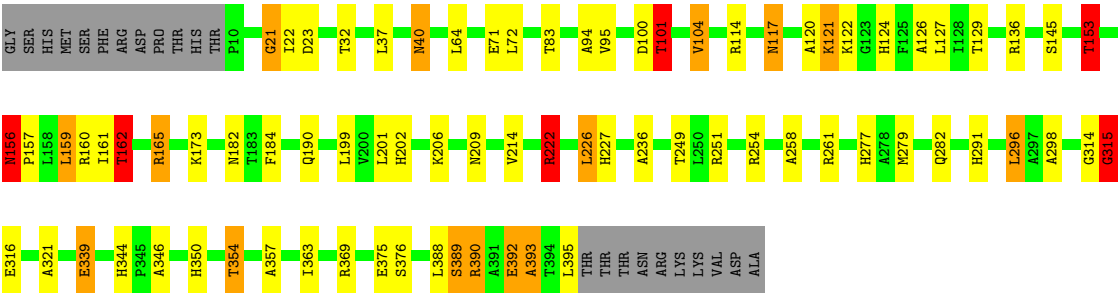
• Molecule 1: Cystathionine gamma-synthase

Chain C: 





● Molecule 1: Cystathionine gamma-synthase



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	165.42Å 165.42Å 241.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.10 48.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.80-2.10) 99.9 (48.80-2.10)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.162 , 0.190 0.169 , 0.195	Depositor DCC
R_{free} test set	9421 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$ 0.004 for $-1/2^*h-1/2^*k-1/2^*l, -1/2^*h-1/2^*k+1/2^*l, -h+k$ 0.000 for $-1/2^*h+1/2^*k+1/2^*l, 1/2^*h-1/2^*k+1/2^*l, h+k$ 0.002 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.487 for $h, -k, -l$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12288	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 2.81% 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: LLP, PGE, PEG

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	1.50	23/2926 (0.8%)	1.58	32/3982 (0.8%)
1	B	1.50	29/2910 (1.0%)	1.62	33/3959 (0.8%)
1	C	1.50	27/2924 (0.9%)	1.62	35/3979 (0.9%)
1	D	1.49	20/2919 (0.7%)	1.60	30/3971 (0.8%)
All	All	1.50	99/11679 (0.8%)	1.60	130/15891 (0.8%)

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
1	B	0	4
1	C	0	2
1	D	0	3
All	All	0	10

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	145	SER	CA-CB	-8.72	1.46	1.52
1	B	257	ASP	CG-OD2	8.67	1.41	1.25
1	D	83	THR	C-O	8.54	1.34	1.23
1	D	339	GLU	CD-OE2	8.33	1.41	1.25
1	C	257	ASP	CG-OD2	8.23	1.41	1.25
1	A	114	ARG	NE-CZ	8.23	1.42	1.33
1	A	10	PRO	C-O	-8.13	1.13	1.24
1	C	114	ARG	NE-CZ	7.89	1.41	1.33
1	C	64	LEU	C-O	-7.83	1.15	1.24
1	B	275	ASP	C-O	7.54	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	22	ILE	C-O	-7.51	1.15	1.24
1	A	83	THR	C-O	7.50	1.33	1.23
1	A	222	ARG	C-O	-7.28	1.15	1.24
1	A	22	ILE	C-O	-7.19	1.15	1.24
1	C	333	GLU	C-O	7.18	1.33	1.23
1	B	339	GLU	CD-OE2	6.78	1.38	1.25
1	C	282	GLN	C-O	6.68	1.32	1.23
1	B	333	GLU	C-O	6.58	1.32	1.23
1	D	64	LEU	C-O	-6.57	1.16	1.24
1	B	329	PHE	C-O	-6.54	1.16	1.24
1	B	202	HIS	CE1-NE2	6.49	1.39	1.32
1	A	145	SER	CA-CB	-6.48	1.48	1.52
1	C	211	HIS	CE1-NE2	6.39	1.39	1.32
1	C	190	GLN	C-O	6.35	1.31	1.23
1	C	54	TYR	C-O	6.35	1.31	1.23
1	C	175	GLY	C-O	-6.33	1.15	1.23
1	A	291	HIS	CE1-NE2	6.32	1.38	1.32
1	A	182	ASN	C-O	6.29	1.32	1.24
1	B	281	ASN	C-O	-6.21	1.16	1.24
1	A	275	ASP	C-O	-6.15	1.16	1.24
1	D	375	GLU	C-O	6.14	1.32	1.23
1	C	152	GLU	C-O	6.12	1.30	1.23
1	A	339	GLU	CD-OE2	6.12	1.36	1.25
1	A	77	GLY	C-O	6.08	1.30	1.23
1	D	258	ALA	C-O	6.07	1.31	1.24
1	B	175	GLY	C-O	-6.03	1.16	1.24
1	D	315	GLY	C-O	6.03	1.29	1.23
1	A	258	ALA	C-O	5.96	1.31	1.24
1	A	127	LEU	N-CA	5.93	1.53	1.46
1	C	62	ARG	CD-NE	-5.89	1.38	1.46
1	C	77	GLY	C-O	5.87	1.30	1.24
1	B	64	LEU	C-O	-5.86	1.17	1.24
1	D	121	LYS	C-O	-5.84	1.16	1.24
1	A	71	GLU	C-O	-5.83	1.17	1.24
1	D	156	ASN	C-O	-5.78	1.18	1.25
1	B	62	ARG	CD-NE	-5.74	1.38	1.46
1	D	71	GLU	C-O	-5.74	1.17	1.24
1	B	143	ALA	C-O	-5.72	1.16	1.24
1	B	298	ALA	C-O	-5.64	1.17	1.24
1	A	130	ALA	C-O	5.63	1.30	1.23
1	A	94	ALA	C-O	-5.63	1.17	1.24
1	C	133	THR	C-O	-5.60	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	VAL	C-O	-5.60	1.18	1.23
1	B	211	HIS	CE1-NE2	5.59	1.38	1.32
1	B	276	GLY	CA-C	5.56	1.59	1.51
1	A	156	ASN	C-O	-5.55	1.18	1.25
1	A	278	ALA	C-O	-5.50	1.17	1.24
1	A	294	HIS	CE1-NE2	5.49	1.38	1.32
1	D	37	LEU	C-O	5.45	1.31	1.24
1	B	249	THR	C-O	-5.42	1.17	1.24
1	D	376[A]	SER	C-O	5.41	1.30	1.23
1	D	376[B]	SER	C-O	5.41	1.30	1.23
1	D	214	VAL	C-O	5.39	1.29	1.24
1	C	390	ARG	C-O	5.38	1.30	1.24
1	B	222	ARG	NE-CZ	5.34	1.39	1.33
1	C	114	ARG	CZ-NH1	5.33	1.40	1.32
1	D	222	ARG	C-O	-5.32	1.17	1.24
1	D	23	ASP	CG-OD1	5.31	1.35	1.25
1	D	298	ALA	C-O	-5.31	1.17	1.24
1	A	23	ASP	CG-OD1	5.27	1.35	1.25
1	B	289	ALA	C-O	-5.26	1.17	1.24
1	C	289	ALA	C-O	-5.26	1.17	1.24
1	C	83	THR	C-O	5.25	1.30	1.23
1	C	281	ASN	C-O	-5.25	1.17	1.24
1	B	72	LEU	C-O	-5.24	1.17	1.24
1	D	227	HIS	CE1-NE2	5.23	1.37	1.32
1	B	173	LYS	C-O	-5.23	1.17	1.24
1	C	166	PHE	C-O	5.20	1.30	1.24
1	C	21	GLY	CA-C	5.20	1.59	1.51
1	C	202	HIS	CE1-NE2	5.20	1.37	1.32
1	B	54	TYR	C-O	5.20	1.30	1.23
1	B	103	VAL	C-O	-5.19	1.18	1.24
1	B	63	ASP	C-O	-5.18	1.18	1.24
1	A	129	THR	C-O	-5.17	1.17	1.24
1	C	76	ALA	C-O	-5.15	1.17	1.24
1	D	94	ALA	C-O	-5.14	1.17	1.24
1	C	339	GLU	CD-OE2	5.14	1.35	1.25
1	B	373	GLY	C-O	5.13	1.28	1.23
1	C	278	ALA	C-O	-5.11	1.17	1.24
1	B	282	GLN	C-O	5.07	1.30	1.23
1	A	227	HIS	CE1-NE2	5.07	1.37	1.32
1	A	114	ARG	CZ-NH2	5.07	1.40	1.33
1	C	173	LYS	C-O	-5.05	1.17	1.24
1	B	349	THR	C-O	-5.03	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	349	THR	C-O	-5.03	1.17	1.24
1	B	190	GLN	C-O	5.03	1.30	1.23
1	B	331	LEU	C-O	5.02	1.29	1.23
1	C	276	GLY	C-O	-5.01	1.17	1.24
1	B	194	ASP	C-O	-5.00	1.17	1.24

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	153	THR	CB-CA-C	-12.73	90.11	109.20
1	D	153	THR	CB-CA-C	-11.95	91.28	109.20
1	C	55	THR	CA-CB-OG1	11.68	127.12	109.60
1	D	153	THR	CA-CB-OG1	11.44	126.77	109.60
1	D	390	ARG	NE-CZ-NH2	-10.97	109.32	119.20
1	B	55	THR	CA-CB-OG1	10.56	125.43	109.60
1	A	114	ARG	NE-CZ-NH2	10.35	128.51	119.20
1	C	390	ARG	NE-CZ-NH2	-9.76	110.42	119.20
1	C	153	THR	CA-CB-OG1	9.64	124.06	109.60
1	C	114	ARG	NE-CZ-NH2	-9.56	110.60	119.20
1	A	339	GLU	CB-CG-CD	9.52	128.79	112.60
1	C	114	ARG	NE-CZ-NH1	9.50	131.00	121.50
1	C	249	THR	CA-CB-OG1	9.32	123.58	109.60
1	B	55	THR	N-CA-CB	9.00	124.08	110.22
1	B	390	ARG	NE-CZ-NH2	-8.91	111.18	119.20
1	B	165	ARG	CG-CD-NE	-8.84	92.56	112.00
1	D	32	THR	CA-CB-OG1	-8.80	96.40	109.60
1	B	205	THR	CA-CB-OG1	8.50	122.36	109.60
1	D	162	THR	CA-CB-OG1	8.23	121.94	109.60
1	C	55	THR	N-CA-CB	8.09	122.67	110.22
1	C	390	ARG	CG-CD-NE	-8.04	94.32	112.00
1	D	390	ARG	NE-CZ-NH1	8.00	129.50	121.50
1	C	390	ARG	CD-NE-CZ	7.81	135.33	124.40
1	B	390	ARG	CG-CD-NE	-7.56	95.38	112.00
1	D	129	THR	CA-CB-OG1	-7.52	98.32	109.60
1	A	114	ARG	CG-CD-NE	7.47	128.43	112.00
1	D	390	ARG	CD-NE-CZ	7.45	134.83	124.40
1	D	23	ASP	CB-CA-C	7.45	122.30	111.73
1	C	314	GLY	CA-C-N	-7.44	111.69	121.96
1	C	314	GLY	C-N-CA	-7.44	111.69	121.96
1	B	395	LEU	CA-C-O	-7.39	108.24	120.80
1	A	114	ARG	NE-CZ-NH1	-7.33	114.17	121.50
1	C	390	ARG	NE-CZ-NH1	7.28	128.78	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	389	SER	N-CA-CB	7.23	120.49	110.01
1	C	114	ARG	CD-NE-CZ	7.20	134.49	124.40
1	C	20	ALA	O-C-N	-7.20	114.03	122.95
1	A	162	THR	CA-CB-OG1	7.16	120.34	109.60
1	B	390	ARG	CD-NE-CZ	7.09	134.32	124.40
1	A	23	ASP	CB-CA-C	7.01	121.85	111.89
1	D	114	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	A	223	ASP	CA-CB-CG	6.83	119.43	112.60
1	A	100	ASP	CA-CB-CG	6.75	119.35	112.60
1	B	129	THR	CA-CB-OG1	-6.71	99.54	109.60
1	A	101	THR	CB-CA-C	6.70	122.54	109.33
1	C	129	THR	CA-CB-OG1	-6.68	99.58	109.60
1	A	261	ARG	CB-CG-CD	-6.64	96.03	111.30
1	D	222	ARG	CG-CD-NE	-6.54	97.60	112.00
1	A	389	SER	N-CA-CB	6.52	119.71	110.12
1	C	32	THR	CA-CB-OG1	-6.49	99.87	109.60
1	D	261	ARG	CB-CG-CD	-6.44	96.48	111.30
1	C	55	THR	CA-C-O	-6.43	112.83	120.10
1	A	32	THR	CA-CB-OG1	-6.39	100.01	109.60
1	B	129	THR	CB-CA-C	6.38	120.21	109.48
1	A	222	ARG	CA-C-O	-6.38	114.12	120.82
1	B	241	GLY	CA-C-N	6.34	129.16	120.67
1	B	241	GLY	C-N-CA	6.34	129.16	120.67
1	C	129	THR	CB-CA-C	6.30	120.07	109.48
1	A	395	LEU	CA-C-O	-6.24	110.20	120.80
1	B	32	THR	CB-CA-C	6.24	116.98	109.31
1	A	11	CYS	N-CA-C	-6.19	101.03	110.14
1	A	95	VAL	CA-C-O	-6.17	114.50	120.30
1	D	388	LEU	CA-C-O	-6.17	113.88	120.42
1	D	100	ASP	CA-CB-CG	6.13	118.73	112.60
1	D	314	GLY	O-C-N	-6.10	117.66	122.90
1	C	249	THR	N-CA-CB	6.08	119.15	110.16
1	D	390	ARG	CG-CD-NE	-6.05	98.69	112.00
1	B	162	THR	CA-CB-OG1	5.97	118.56	109.60
1	C	394	THR	CB-CA-C	5.97	122.30	110.42
1	B	390	ARG	NE-CZ-NH1	5.87	127.36	121.50
1	C	56	ARG	N-CA-C	-5.84	104.99	111.71
1	D	101	THR	CB-CA-C	5.82	120.49	109.37
1	B	18	VAL	CA-C-O	-5.80	114.70	120.85
1	A	157	PRO	N-CA-CB	-5.79	96.23	102.60
1	A	20	ALA	O-C-N	-5.76	115.81	122.95
1	B	327	ARG	CG-CD-NE	5.73	124.61	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	109	TYR	CA-C-N	5.71	126.43	120.03
1	C	109	TYR	C-N-CA	5.71	126.43	120.03
1	B	254	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	D	95	VAL	CA-C-O	-5.67	114.97	120.30
1	C	385	ARG	CG-CD-NE	-5.66	99.55	112.00
1	B	388	LEU	CA-C-O	-5.65	114.56	120.55
1	C	114	ARG	CG-CD-NE	5.64	124.41	112.00
1	D	296	LEU	N-CA-CB	-5.63	101.84	110.12
1	D	222	ARG	NE-CZ-NH2	-5.62	114.14	119.20
1	D	165	ARG	CB-CG-CD	5.59	124.15	111.30
1	B	114	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	A	292	PRO	CB-CA-C	-5.54	104.51	111.71
1	D	392	GLU	N-CA-C	-5.49	102.27	110.23
1	D	104	VAL	N-CA-CB	-5.47	103.55	111.21
1	B	324	ASP	CA-C-N	-5.46	110.70	121.41
1	B	324	ASP	C-N-CA	-5.46	110.70	121.41
1	A	394	THR	N-CA-CB	-5.44	101.29	110.49
1	C	364	SER	N-CA-CB	-5.44	102.17	110.45
1	A	129	THR	CA-CB-OG1	-5.44	101.44	109.60
1	B	10	PRO	CA-C-N	5.43	132.06	122.67
1	B	10	PRO	C-N-CA	5.43	132.06	122.67
1	A	57	SER	CB-CA-C	5.42	118.73	109.24
1	A	324	ASP	CA-C-N	-5.40	110.83	121.41
1	A	324	ASP	C-N-CA	-5.40	110.83	121.41
1	D	117	ASN	CA-CB-CG	-5.39	107.21	112.60
1	B	327	ARG	CB-CG-CD	-5.38	98.92	111.30
1	A	364	SER	CA-C-N	5.37	128.01	120.28
1	A	364	SER	C-N-CA	5.37	128.01	120.28
1	A	351	ALA	CA-C-N	5.31	127.71	120.54
1	A	351	ALA	C-N-CA	5.31	127.71	120.54
1	C	156	ASN	CA-CB-CG	-5.31	107.29	112.60
1	B	389	SER	N-CA-CB	5.29	117.73	110.07
1	B	55	THR	CA-C-O	-5.22	114.20	120.10
1	B	62	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	C	55	THR	OG1-CB-CG2	5.20	119.69	109.30
1	D	71	GLU	CB-CG-CD	5.18	121.42	112.60
1	B	55	THR	OG1-CB-CG2	5.17	119.65	109.30
1	D	222	ARG	CA-C-O	-5.16	114.95	120.42
1	D	120	ALA	CA-C-O	-5.15	114.96	120.42
1	A	129	THR	CB-CA-C	5.15	118.24	109.75
1	B	91	VAL	CA-C-O	-5.14	115.72	121.17
1	A	388	LEU	CA-C-O	-5.13	115.11	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	18	VAL	O-C-N	5.13	127.11	121.83
1	B	19	ARG	CB-CG-CD	5.12	123.06	111.30
1	C	222	ARG	CD-NE-CZ	5.08	131.52	124.40
1	A	11	CYS	CA-C-O	-5.06	115.30	121.78
1	C	261	ARG	CB-CG-CD	-5.05	99.68	111.30
1	B	213	ASP	CA-CB-CG	5.05	117.65	112.60
1	D	314	GLY	CA-C-N	-5.04	112.50	121.48
1	D	314	GLY	C-N-CA	-5.04	112.50	121.48
1	C	11	CYS	CA-C-O	-5.03	115.50	121.89
1	C	62	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	C	222	ARG	NE-CZ-NH1	5.02	126.52	121.50
1	C	358	ARG	N-CA-C	-5.01	105.73	111.14
1	A	23	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	HIS	Peptide
1	B	202	HIS	Peptide
1	B	21	GLY	Peptide
1	B	276	GLY	Peptide
1	B	44	ASP	Peptide
1	C	202	HIS	Peptide
1	C	315	GLY	Peptide
1	D	202	HIS	Peptide
1	D	21	GLY	Peptide
1	D	315	GLY	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	2891	0	2886	36	0
1	B	2878	0	2873	52	0
1	C	2892	0	2879	35	0
1	D	2884	0	2880	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	7	0	10	1	0
2	D	14	0	20	0	0
3	B	30	0	42	6	0
3	C	10	0	14	0	0
3	D	10	0	14	0	0
4	A	146	0	0	7	0
4	B	187	0	0	12	0
4	C	176	0	0	2	0
4	D	163	0	0	6	0
All	All	12288	0	11618	160	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 (160) 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:223:ASP:HB2	4:A:724:HOH:O	1.60	1.01
1:D:153:THR:HG23	1:D:162:THR:H	1.36	0.90
1:D:277:HIS:HD2	1:D:279:MET:H	1.20	0.89
1:D:315:GLY:HA3	4:D:747:HOH:O	1.72	0.88
1:C:153:THR:HG23	1:C:162:THR:H	1.38	0.86
1:A:394:THR:O	1:A:395:LEU:HB2	1.78	0.83
1:D:354:THR:HG23	1:D:357:ALA:CB	2.10	0.82
1:D:354:THR:HG23	1:D:357:ALA:HB2	1.62	0.81
1:C:251:ARG:HH22	1:D:209:ASN:HD21	1.28	0.81
1:A:113:TRP:CZ2	1:A:117:ASN:ND2	2.49	0.80
1:B:205:THR:HG22	1:B:216:GLY:H	1.47	0.79
1:D:21:GLY:H	1:D:254:ARG:HH12	1.29	0.79
1:D:153:THR:CG2	1:D:162:THR:H	1.96	0.77
1:B:277:HIS:HD2	1:B:279:MET:H	1.30	0.76
1:D:392:GLU:O	1:D:393:ALA:CB	2.33	0.75
1:C:153:THR:CG2	1:C:162:THR:H	1.99	0.74
1:A:251:ARG:HH22	1:B:209:ASN:HD21	1.35	0.73
1:A:113:TRP:CH2	1:A:117:ASN:ND2	2.56	0.72
1:A:209:ASN:HD21	1:B:251:ARG:HH22	1.37	0.71
1:B:101:THR:HG23	4:B:631:HOH:O	1.90	0.71
1:C:245:ASP:O	1:C:249:THR:HG23	1.90	0.71
1:A:339:GLU:HG2	1:B:22:ILE:HD12	1.73	0.71
1:B:203:SER:OG	1:B:205:THR:HG23	1.91	0.71
1:D:156:ASN:HD21	1:D:369:ARG:HH11	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ALA:O	1:A:394:THR:HB	1.93	0.68
1:D:321:ALA:O	1:D:390:ARG:HD2	1.94	0.68
1:C:209:ASN:HD21	1:D:251:ARG:HH22	1.39	0.68
1:A:156:ASN:HD21	1:A:369:ARG:HH11	1.42	0.67
1:A:394:THR:O	1:A:395:LEU:CB	2.42	0.67
1:B:321:ALA:O	1:B:390:ARG:HD2	1.94	0.67
1:B:101:THR:HG21	4:B:781:HOH:O	1.93	0.67
1:D:392:GLU:O	1:D:393:ALA:HB3	1.93	0.67
1:C:251:ARG:NH2	1:D:209:ASN:HD21	1.91	0.67
1:C:321:ALA:O	1:C:390:ARG:HD2	1.95	0.67
1:B:229:GLN:HG2	3:B:502:PGE:H22	1.77	0.67
1:D:222:ARG:HG2	1:D:222:ARG:HH11	1.59	0.66
1:D:222:ARG:O	1:D:222:ARG:HG3	1.88	0.66
1:C:38:SER:O	1:C:55:THR:CG2	2.45	0.65
1:D:201:LEU:HD12	1:D:201:LEU:C	2.22	0.64
1:C:156:ASN:HB2	1:C:184:PHE:CZ	2.32	0.64
1:A:201:LEU:HD12	1:A:201:LEU:C	2.22	0.64
1:A:162:THR:HG21	4:A:722:HOH:O	1.99	0.63
1:C:209:ASN:HD22	1:C:249:THR:HA	1.65	0.61
1:D:162:THR:HG21	4:D:729:HOH:O	1.99	0.61
1:C:38:SER:O	1:C:55:THR:HG21	2.02	0.60
1:D:389:SER:O	1:D:392:GLU:O	2.18	0.60
1:D:40:ASN:HD22	1:D:40:ASN:H	1.49	0.60
1:A:282:GLN:NE2	4:A:603:HOH:O	2.33	0.60
1:B:38:SER:O	1:B:55:THR:CG2	2.49	0.60
1:A:394:THR:CG2	4:A:609:HOH:O	2.51	0.59
1:A:209:ASN:HD21	1:B:251:ARG:NH2	2.00	0.58
1:D:222:ARG:HG2	1:D:222:ARG:NH1	2.18	0.58
1:A:339:GLU:CG	1:B:22:ILE:HD12	2.32	0.58
1:B:209:ASN:HD22	1:B:249:THR:HA	1.68	0.58
1:B:162:THR:HG21	4:B:766:HOH:O	2.03	0.57
1:B:55:THR:CG2	1:B:59:ASN:HD22	2.17	0.57
1:D:277:HIS:CD2	1:D:279:MET:H	2.11	0.57
1:C:9:THR:O	1:C:10:PRO:O	2.23	0.57
1:B:156:ASN:HD21	1:B:369:ARG:HH11	1.53	0.57
1:B:275:ASP:O	1:B:276:GLY:C	2.48	0.57
1:A:40:ASN:HD22	1:A:40:ASN:H	1.54	0.56
1:B:156:ASN:ND2	1:B:369:ARG:HH11	2.03	0.55
3:B:501:PGE:H4	4:B:778:HOH:O	2.06	0.55
1:A:251:ARG:NH2	1:B:209:ASN:HD21	2.02	0.55
1:B:38:SER:O	1:B:55:THR:HG21	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASN:ND2	1:C:369:ARG:HH11	2.05	0.55
1:C:21:GLY:HA2	1:C:24:ARG:CG	2.37	0.54
1:D:40:ASN:HD22	1:D:40:ASN:N	2.05	0.54
1:B:66:GLY:N	1:B:80:ILE:HD11	2.22	0.54
1:D:291:HIS:HD2	4:D:651:HOH:O	1.90	0.54
1:B:21:GLY:N	1:B:254:ARG:HH12	2.06	0.53
3:B:501:PGE:C4	4:B:778:HOH:O	2.56	0.53
1:D:159:LEU:O	1:D:291:HIS:HE1	1.91	0.53
1:B:121:LYS:HG2	3:B:503:PGE:H6	1.91	0.53
1:C:21:GLY:HA2	1:C:24:ARG:HG2	1.91	0.52
1:B:165:ARG:NE	4:B:604:HOH:O	2.41	0.52
1:A:21:GLY:H	1:A:24:ARG:NH2	2.08	0.52
1:D:160:ARG:HH11	1:D:160:ARG:HG3	1.75	0.52
1:B:156:ASN:HB2	1:B:184:PHE:CZ	2.44	0.51
1:A:101:THR:HB	1:A:126:ALA:HB3	1.91	0.51
1:C:209:ASN:HD21	1:D:251:ARG:NH2	2.06	0.51
1:D:162:THR:CG2	4:D:697:HOH:O	2.58	0.51
1:A:162:THR:CG2	4:A:693:HOH:O	2.58	0.50
1:D:354:THR:HG23	1:D:357:ALA:HB3	1.91	0.50
1:D:156:ASN:HD22	1:D:157:PRO:CA	2.24	0.50
1:B:124:HIS:HE1	4:C:695:HOH:O	1.95	0.50
1:B:66:GLY:N	1:B:80:ILE:CD1	2.75	0.50
1:B:21:GLY:H	1:B:254:ARG:HH12	1.58	0.50
1:D:209:ASN:HD22	1:D:249:THR:HA	1.77	0.49
1:B:205:THR:CG2	1:B:206:LLP:OP1	2.61	0.49
1:D:153:THR:HG23	1:D:162:THR:N	2.16	0.49
4:A:681:HOH:O	1:D:124:HIS:HE1	1.96	0.49
1:A:40:ASN:HD22	1:A:40:ASN:N	2.11	0.49
1:A:109:TYR:OH	2:A:501:PEG:H21	2.14	0.48
1:A:156:ASN:HD22	1:A:157:PRO:CA	2.26	0.48
1:C:55:THR:CG2	1:C:59:ASN:HD22	2.26	0.48
1:A:156:ASN:HD22	1:A:156:ASN:C	2.21	0.48
1:C:156:ASN:HD21	1:C:369:ARG:HH11	1.62	0.48
1:B:162:THR:CG2	4:B:716:HOH:O	2.62	0.47
1:B:206:LLP:HD3	1:B:335:LEU:HG	1.96	0.47
1:A:113:TRP:CE2	1:A:117:ASN:ND2	2.83	0.47
1:D:354:THR:CG2	1:D:357:ALA:HB2	2.40	0.47
1:C:159:LEU:O	1:C:291:HIS:HE1	1.97	0.47
1:C:199:LEU:HD21	1:C:226:LEU:HD13	1.96	0.47
1:A:209:ASN:HD22	1:A:249:THR:HA	1.79	0.47
1:D:282:GLN:NE2	4:D:605:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASP:HB2	1:A:296:LEU:HD11	1.96	0.47
1:B:55:THR:HG21	1:B:59:ASN:HD22	1.80	0.47
1:A:162:THR:HG23	4:A:693:HOH:O	2.15	0.46
1:B:55:THR:HB	1:B:59:ASN:HB2	1.97	0.46
4:B:713:HOH:O	1:C:124:HIS:HE1	1.98	0.46
1:B:24:ARG:HH11	1:B:24:ARG:CG	2.28	0.46
1:B:203:SER:HG	1:B:205:THR:HG23	1.80	0.46
1:C:9:THR:C	1:C:10:PRO:O	2.59	0.46
1:B:122:LYS:NZ	4:B:603:HOH:O	2.40	0.45
1:B:229:GLN:HG2	3:B:502:PGE:C2	2.46	0.45
1:C:201:LEU:C	1:C:201:LEU:HD12	2.42	0.45
1:D:162:THR:HG23	4:D:697:HOH:O	2.16	0.45
1:C:393:ALA:C	1:C:394:THR:O	2.56	0.45
1:C:309:SER:HB3	1:C:367:LEU:HD11	1.99	0.44
1:D:101:THR:HA	1:D:126:ALA:O	2.18	0.44
1:D:156:ASN:HD22	1:D:156:ASN:C	2.25	0.44
1:C:122:LYS:NZ	4:C:602:HOH:O	2.33	0.44
1:D:222:ARG:CZ	1:D:222:ARG:CB	2.94	0.44
1:B:38:SER:O	1:B:55:THR:HG23	2.18	0.44
1:D:199:LEU:HD21	1:D:226:LEU:HD13	1.98	0.44
1:B:106:HIS:HE1	4:B:759:HOH:O	2.00	0.44
1:C:21:GLY:H	1:C:24:ARG:CZ	2.31	0.44
1:C:153:THR:CG2	1:C:161:ILE:HA	2.47	0.44
1:D:153:THR:CG2	1:D:161:ILE:HA	2.48	0.44
1:B:153:THR:HB	1:B:162:THR:HG23	2.00	0.43
1:B:162:THR:HG22	4:B:716:HOH:O	2.17	0.43
1:A:126:ALA:O	1:A:127:LEU:HB2	2.18	0.43
1:B:101:THR:CG2	4:B:631:HOH:O	2.59	0.43
1:C:44:ASP:O	1:C:48:ASN:HB2	2.19	0.43
1:A:114:ARG:NH2	1:D:236:ALA:HA	2.33	0.43
1:B:339:GLU:CD	1:B:339:GLU:H	2.27	0.43
1:A:257:ASP:O	1:A:261:ARG:HG3	2.19	0.42
1:A:93:ASN:O	1:D:122:LYS:NZ	2.49	0.42
1:B:199:LEU:HD21	1:B:226:LEU:HD13	2.01	0.42
1:D:182:ASN:HD21	1:D:190:GLN:HB3	1.84	0.42
1:A:206:LLP:HD3	1:A:335:LEU:HG	2.01	0.42
1:D:156:ASN:HA	1:D:157:PRO:HA	1.88	0.42
1:A:33:PRO:HA	1:A:34:PRO:HD3	1.86	0.42
1:D:344:HIS:CE1	1:D:346:ALA:HB3	2.55	0.41
1:B:201:LEU:C	1:B:201:LEU:HD12	2.44	0.41
1:B:205:THR:HG21	1:B:206:LLP:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLU:CD	1:A:339:GLU:H	2.29	0.41
1:B:185:LEU:HB3	1:B:189:LEU:HB2	2.02	0.41
1:B:205:THR:HB	1:B:214:VAL:O	2.20	0.41
1:B:229:GLN:HG2	3:B:502:PGE:C1	2.50	0.41
1:C:22:ILE:HA	1:C:31:VAL:O	2.21	0.41
1:C:101:THR:HG21	1:C:128:ILE:CD1	2.51	0.41
1:C:207:TYR:CE1	1:C:336:GLY:HA2	2.57	0.40
1:C:38:SER:O	1:C:55:THR:HG23	2.17	0.40
1:B:22:ILE:HA	1:B:31:VAL:O	2.21	0.40
1:B:33:PRO:HA	1:B:34:PRO:HD3	1.94	0.40
1:C:153:THR:HG22	1:C:154:PRO:HA	2.04	0.40
1:C:339:GLU:H	1:C:339:GLU:CD	2.29	0.40
1:D:350:HIS:CD2	1:D:363:ILE:CD1	3.05	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	386/408 (95%)	374 (97%)	10 (3%)	2 (0%)	24	22
1	B	384/408 (94%)	375 (98%)	7 (2%)	2 (0%)	24	22
1	C	386/408 (95%)	374 (97%)	7 (2%)	5 (1%)	9	6
1	D	385/408 (94%)	375 (97%)	9 (2%)	1 (0%)	36	36
All	All	1541/1632 (94%)	1498 (97%)	33 (2%)	10 (1%)	18	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	10	PRO
1	C	394	THR

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Mol	Chain	Res	Type
1	D	393	ALA
1	A	324	ASP
1	A	353	MET
1	C	395	LEU
1	B	324	ASP
1	C	324	ASP
1	B	276	GLY
1	C	21	GLY

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	292/309 (94%)	271 (93%)	21 (7%)	13	11
1	B	289/309 (94%)	271 (94%)	18 (6%)	16	14
1	C	291/309 (94%)	271 (93%)	20 (7%)	14	12
1	D	291/309 (94%)	269 (92%)	22 (8%)	12	9
All	All	1163/1236 (94%)	1082 (93%)	81 (7%)	14	11

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	40	ASN
1	A	57	SER
1	A	72	LEU
1	A	101	THR
1	A	114	ARG
1	A	127	LEU
1	A	136	ARG
1	A	156	ASN
1	A	157	PRO
1	A	160	ARG
1	A	162	THR
1	A	165	ARG

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Mol	Chain	Res	Type
1	A	173	LYS
1	A	184	PHE
1	A	253	LEU
1	A	273	LEU
1	A	296	LEU
1	A	339	GLU
1	A	353	MET
1	A	394	THR
1	B	24	ARG
1	B	55	THR
1	B	72	LEU
1	B	101	THR
1	B	121	LYS
1	B	129	THR
1	B	157	PRO
1	B	162	THR
1	B	184	PHE
1	B	205	THR
1	B	223	ASP
1	B	226	LEU
1	B	253	LEU
1	B	273	LEU
1	B	299	ARG
1	B	333	GLU
1	B	339	GLU
1	B	395	LEU
1	C	24	ARG
1	C	32	THR
1	C	55	THR
1	C	57	SER
1	C	72	LEU
1	C	114	ARG
1	C	121	LYS
1	C	129	THR
1	C	153	THR
1	C	159	LEU
1	C	160	ARG
1	C	173	LYS
1	C	184	PHE
1	C	226	LEU
1	C	249	THR
1	C	253	LEU

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Mol	Chain	Res	Type
1	C	272	GLU
1	C	333	GLU
1	C	339	GLU
1	C	356	GLU
1	D	40	ASN
1	D	72	LEU
1	D	101	THR
1	D	104	VAL
1	D	117	ASN
1	D	121	LYS
1	D	127	LEU
1	D	136	ARG
1	D	153	THR
1	D	156	ASN
1	D	159	LEU
1	D	162	THR
1	D	165	ARG
1	D	173	LYS
1	D	184	PHE
1	D	222	ARG
1	D	226	LEU
1	D	296	LEU
1	D	316	GLU
1	D	339	GLU
1	D	354	THR
1	D	395	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	97	GLN
1	A	156	ASN
1	A	182	ASN
1	A	209	ASN
1	A	301	GLN
1	B	124	HIS
1	B	156	ASN
1	B	182	ASN
1	B	209	ASN
1	B	229	GLN
1	B	277	HIS

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Mol	Chain	Res	Type
1	B	282	GLN
1	C	51	GLN
1	C	124	HIS
1	C	156	ASN
1	C	182	ASN
1	C	209	ASN
1	C	291	HIS
1	D	40	ASN
1	D	89	ASN
1	D	97	GLN
1	D	124	HIS
1	D	156	ASN
1	D	182	ASN
1	D	209	ASN
1	D	277	HIS
1	D	291	HIS
1	D	301	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
1	LLP	A	206	1	23,24,25	1.29	1 (4%)	25,32,34	1.38	3 (12%)
1	LLP	C	206	1	23,24,25	1.42	3 (13%)	25,32,34	1.19	2 (8%)
1	LLP	B	206	1	23,24,25	1.76	5 (21%)	25,32,34	1.64	4 (16%)
1	LLP	D	206	1	23,24,25	1.33	3 (13%)	25,32,34	1.53	5 (20%)

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
1	LLP	A	206	1	-	6/16/17/19	0/1/1/1
1	LLP	C	206	1	-	5/16/17/19	0/1/1/1
1	LLP	B	206	1	-	5/16/17/19	0/1/1/1
1	LLP	D	206	1	-	5/16/17/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	LLP	C4'-NZ	5.40	1.45	1.27
1	A	206	LLP	C4'-NZ	4.54	1.42	1.27
1	D	206	LLP	C4'-NZ	3.76	1.39	1.27
1	C	206	LLP	C3-C2	-3.69	1.37	1.41
1	B	206	LLP	CD-CE	3.47	1.63	1.51
1	C	206	LLP	C4'-NZ	3.19	1.37	1.27
1	B	206	LLP	C3-C2	-2.68	1.38	1.41
1	B	206	LLP	C4-C4'	2.66	1.52	1.46
1	D	206	LLP	CD-CE	2.28	1.59	1.51
1	C	206	LLP	O3-C3	-2.21	1.31	1.36
1	D	206	LLP	C4-C4'	2.19	1.51	1.46
1	B	206	LLP	O3-C3	-2.12	1.32	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	LLP	C5-C4-C4'	3.78	127.30	121.47
1	B	206	LLP	C4-C3-C2	3.67	122.21	120.14
1	B	206	LLP	C3-C4-C5	-3.48	115.48	118.28
1	A	206	LLP	C5-C4-C4'	3.34	126.62	121.47
1	D	206	LLP	C4-C3-C2	3.28	121.99	120.14
1	D	206	LLP	C5-C4-C4'	2.98	126.06	121.47
1	A	206	LLP	OP4-C5'-C5	2.93	114.84	109.36
1	D	206	LLP	OP4-C5'-C5	2.62	114.28	109.36
1	C	206	LLP	CD-CE-NZ	-2.49	104.25	110.83
1	D	206	LLP	CE-NZ-C4'	2.38	126.35	118.72
1	A	206	LLP	C3-C4-C4'	-2.38	116.10	120.40
1	C	206	LLP	CE-NZ-C4'	2.38	126.33	118.72
1	D	206	LLP	CD-CG-CB	2.11	121.58	113.62
1	B	206	LLP	CE-NZ-C4'	2.02	125.19	118.72

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	206	LLP	O-C-CA-CB
1	B	206	LLP	O-C-CA-CB
1	C	206	LLP	C4-C4'-NZ-CE
1	C	206	LLP	O-C-CA-CB
1	D	206	LLP	O-C-CA-CB
1	B	206	LLP	C4-C4'-NZ-CE
1	D	206	LLP	C4-C4'-NZ-CE
1	A	206	LLP	C4-C4'-NZ-CE
1	A	206	LLP	CG-CD-CE-NZ
1	C	206	LLP	CA-CB-CG-CD
1	D	206	LLP	CG-CD-CE-NZ
1	C	206	LLP	CG-CD-CE-NZ
1	B	206	LLP	C3-C4-C4'-NZ
1	A	206	LLP	CD-CE-NZ-C4'
1	A	206	LLP	C3-C4-C4'-NZ
1	B	206	LLP	CD-CE-NZ-C4'
1	D	206	LLP	C3-C4-C4'-NZ
1	B	206	LLP	CG-CD-CE-NZ
1	C	206	LLP	C-CA-CB-CG
1	D	206	LLP	C-CA-CB-CG
1	A	206	LLP	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	206	LLP	1	0
1	B	206	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	PGE	B	502	-	9,9,9	0.38	0	8,8,8	0.35	0
3	PGE	B	501	-	9,9,9	0.65	0	8,8,8	0.40	0
2	PEG	A	501	-	6,6,6	0.50	0	5,5,5	0.47	0
3	PGE	C	501	-	9,9,9	0.45	0	8,8,8	0.28	0
2	PEG	D	502	-	6,6,6	0.29	0	5,5,5	0.19	0
2	PEG	D	501	-	6,6,6	0.52	0	5,5,5	0.52	0
3	PGE	B	503	-	9,9,9	0.57	0	8,8,8	0.47	0
3	PGE	D	503	-	9,9,9	0.27	0	8,8,8	0.13	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
3	PGE	B	502	-	-	5/7/7/7	-
3	PGE	B	501	-	-	4/7/7/7	-
2	PEG	A	501	-	-	1/4/4/4	-
3	PGE	C	501	-	-	3/7/7/7	-
2	PEG	D	502	-	-	3/4/4/4	-
2	PEG	D	501	-	-	2/4/4/4	-
3	PGE	B	503	-	-	6/7/7/7	-
3	PGE	D	503	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	PGE	C4-C3-O2-C2
3	B	503	PGE	O2-C3-C4-O3
2	D	501	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	D	503	PGE	O2-C3-C4-O3
3	B	501	PGE	O2-C3-C4-O3
3	B	503	PGE	O1-C1-C2-O2
3	B	502	PGE	O2-C3-C4-O3
3	C	501	PGE	O3-C5-C6-O4
2	D	502	PEG	O1-C1-C2-O2
2	D	502	PEG	O2-C3-C4-O4
3	B	503	PGE	O3-C5-C6-O4
3	B	503	PGE	C6-C5-O3-C4
3	C	501	PGE	O2-C3-C4-O3
2	A	501	PEG	C4-C3-O2-C2
3	B	502	PGE	C3-C4-O3-C5
3	D	503	PGE	C6-C5-O3-C4
3	B	501	PGE	O1-C1-C2-O2
3	D	503	PGE	C1-C2-O2-C3
3	B	503	PGE	C3-C4-O3-C5
3	B	503	PGE	C4-C3-O2-C2
3	B	501	PGE	C1-C2-O2-C3
3	B	502	PGE	C6-C5-O3-C4
2	D	501	PEG	O2-C3-C4-O4
3	B	502	PGE	C1-C2-O2-C3
3	B	501	PGE	O3-C5-C6-O4
3	C	501	PGE	C4-C3-O2-C2
2	D	502	PEG	C4-C3-O2-C2
3	D	503	PGE	O3-C5-C6-O4

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	PGE	3	0
3	B	501	PGE	2	0
2	A	501	PEG	1	0
3	B	503	PGE	1	0

5.7 Other polymers ⓘ

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	386/408 (94%)	-1.30	0 100 100	20, 35, 59, 91	2 (0%)
1	B	385/408 (94%)	-1.32	1 (0%) 90 91	23, 32, 52, 97	1 (0%)
1	C	387/408 (94%)	-1.32	2 (0%) 87 88	18, 32, 54, 123	1 (0%)
1	D	385/408 (94%)	-1.29	0 100 100	22, 34, 59, 86	2 (0%)
All	All	1543/1632 (94%)	-1.31	3 (0%) 91 92	18, 34, 56, 123	6 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	PRO	3.7
1	C	10	PRO	3.4
1	C	9	THR	3.0

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
1	LLP	B	206	24/25	0.99	0.04	27,33,38,46	0
1	LLP	C	206	24/25	0.99	0.04	25,35,43,52	0
1	LLP	A	206	24/25	1.00	0.03	26,35,40,46	0
1	LLP	D	206	24/25	1.00	0.04	28,36,45,47	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
3	PGE	B	501	10/10	0.97	0.11	40,83,98,99	0
2	PEG	D	501	7/7	0.98	0.07	44,61,81,81	0
3	PGE	B	503	10/10	0.98	0.08	52,62,69,72	0
3	PGE	C	501	10/10	0.98	0.09	39,83,90,90	0
3	PGE	D	503	10/10	0.98	0.07	53,74,77,79	0
2	PEG	D	502	7/7	0.99	0.06	68,71,79,79	0
2	PEG	A	501	7/7	0.99	0.05	41,54,69,71	0
3	PGE	B	502	10/10	0.99	0.06	56,75,83,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.