



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:37 PM UTC

PDB ID : 3LOY / pdb_00003loy
Title : Crystal structure of a Copper-containing benzylamine oxidase from Hansenula Polymorpha
Authors : Klema, V.J.; Johnson, B.J.; Wilmot, C.M.
Deposited on : 2010-02-04
Resolution : 2.00 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

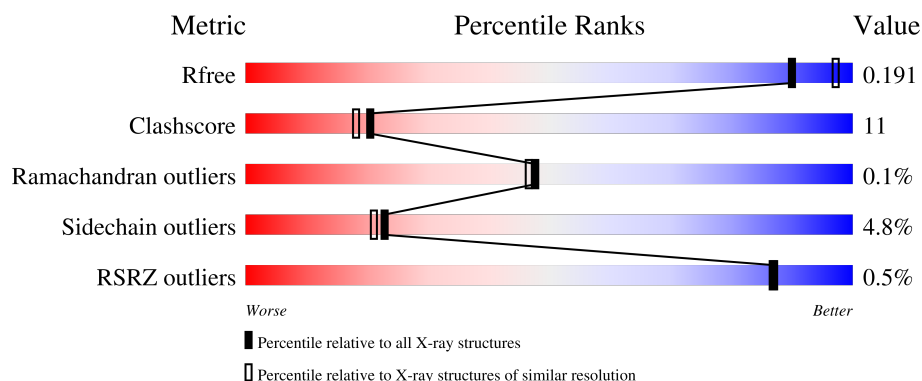
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	633	 82% 15% ..
1	B	633	 77% 19% ..
1	C	633	 81% 15% ..

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	GOL	A	637	-	X	-	-
3	GOL	B	639	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18610 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 copper amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	6	0
			5115	3275	870	944	26			
1	B	633	Total	C	N	O	S	0	6	0
			5120	3276	874	943	27			
1	C	633	Total	C	N	O	S	0	1	0
			5086	3255	867	939	25			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

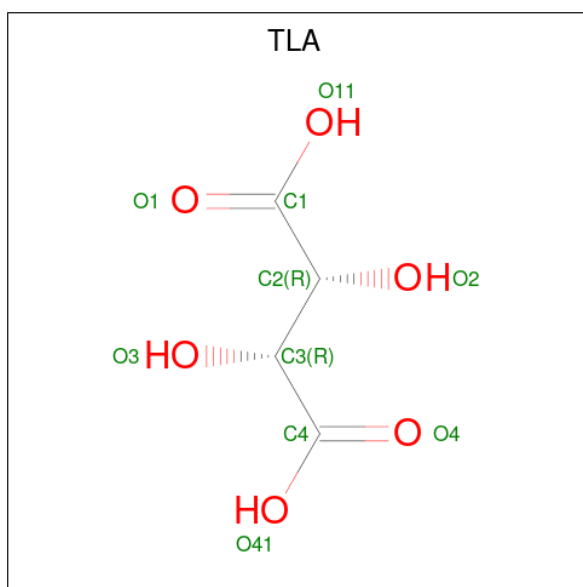
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



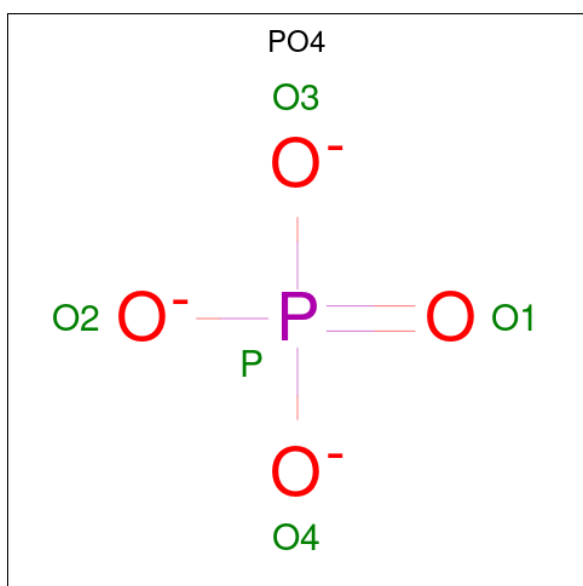
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total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

- Molecule 4 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		

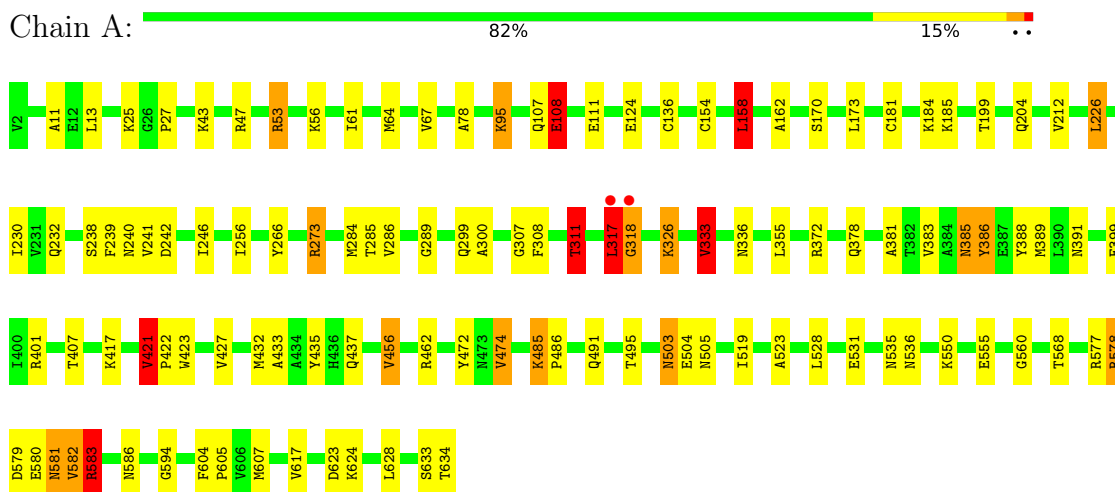
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1028	Total 1028	O 1028	0	0
6	B	1051	Total 1051	O 1051	0	0
6	C	1116	Total 1116	O 1116	0	0

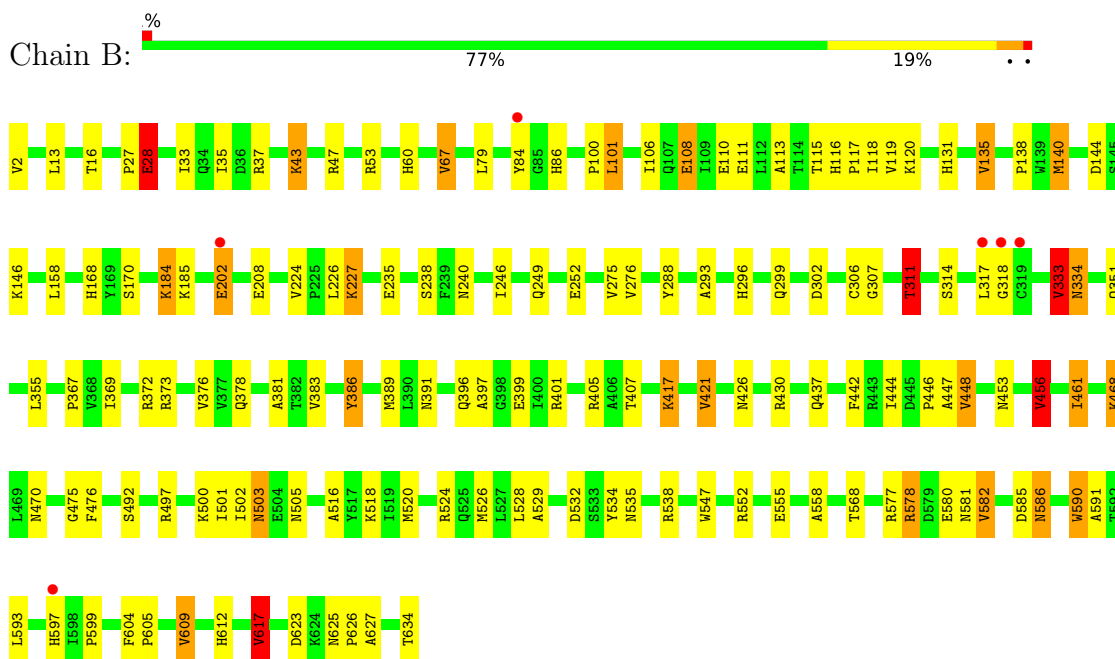
3 Residue-property plots

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: copper amine oxidase



- Molecule 1: copper amine oxidase



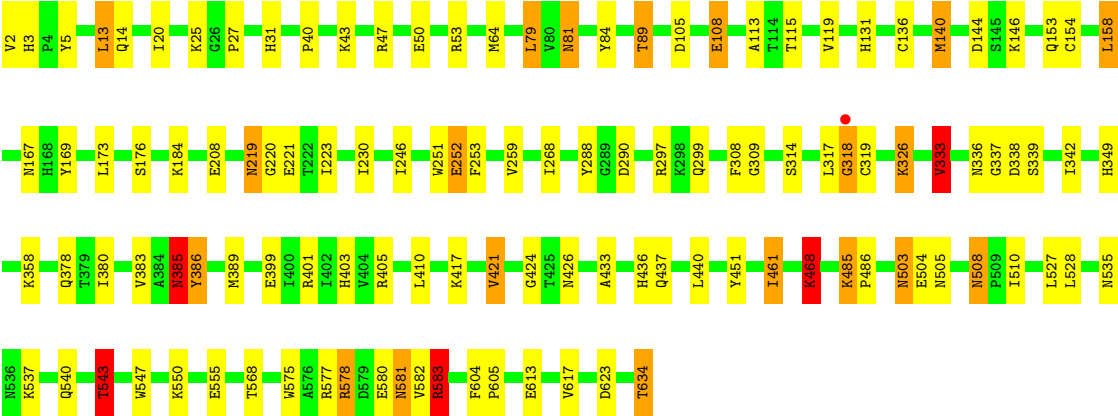
- Molecule 1: copper amine oxidase

Chain C:

81%

15%

..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	288.51Å 91.06Å 151.10Å 90.00° 117.23° 90.00°	Depositor
Resolution (Å)	37.42 – 2.00 37.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.4 (37.42-2.00) 90.4 (37.42-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.145 , 0.191 0.146 , 0.191	Depositor DCC
R_{free} test set	10514 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18610	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: PO4, GOL, CU, TLA, TPQ

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	1.39	21/5253 (0.4%)	1.23	20/7149 (0.3%)
1	B	1.40	11/5255 (0.2%)	1.23	20/7151 (0.3%)
1	C	1.45	10/5212 (0.2%)	1.26	22/7096 (0.3%)
All	All	1.41	42/15720 (0.3%)	1.24	62/21396 (0.3%)

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	2
1	C	0	1
All	All	0	3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	349	HIS	C-O	6.49	1.31	1.23
1	B	448	VAL	CA-CB	6.35	1.61	1.53
1	B	224	VAL	CA-C	-6.00	1.48	1.53
1	B	591	ALA	C-O	6.00	1.31	1.24
1	C	140	MET	SD-CE	5.98	1.94	1.79
1	B	397	ALA	CA-CB	5.97	1.63	1.53
1	B	447	ALA	CA-CB	-5.85	1.48	1.53
1	C	309	GLY	N-CA	5.84	1.53	1.45
1	B	369	ILE	CA-CB	5.82	1.61	1.55
1	A	617	VAL	N-CA	5.72	1.51	1.46
1	A	617	VAL	CA-CB	5.71	1.58	1.54
1	A	266	TYR	C-O	5.71	1.31	1.23
1	A	158	LEU	CA-C	5.54	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	290	ASP	CA-C	5.53	1.59	1.52
1	C	577	ARG	C-O	-5.50	1.16	1.24
1	A	162	ALA	CA-C	5.50	1.60	1.52
1	A	432	MET	CA-C	5.50	1.59	1.52
1	B	442	PHE	C-O	5.46	1.30	1.24
1	B	590	TRP	C-O	5.44	1.30	1.24
1	A	581	ASN	C-O	-5.43	1.17	1.23
1	C	424	GLY	N-CA	5.33	1.51	1.45
1	A	433	ALA	CA-CB	-5.32	1.45	1.53
1	C	358	LYS	C-O	5.32	1.30	1.23
1	A	427	VAL	CA-CB	5.31	1.60	1.54
1	A	617	VAL	C-O	5.30	1.28	1.23
1	B	520	MET	CG-SD	-5.21	1.67	1.80
1	C	223	ILE	CA-C	5.21	1.58	1.52
1	A	594	GLY	CA-C	5.20	1.57	1.52
1	B	501	ILE	C-O	5.18	1.29	1.24
1	A	108	GLU	CB-CG	-5.17	1.36	1.52
1	A	11	ALA	CA-CB	5.16	1.61	1.53
1	A	578	ARG	CD-NE	-5.16	1.39	1.46
1	A	61	ILE	CA-CB	5.14	1.61	1.54
1	A	256	ILE	CA-CB	5.13	1.58	1.54
1	A	422	PRO	CA-C	5.12	1.58	1.52
1	C	468	LYS	CG-CD	5.09	1.67	1.52
1	A	266	TYR	CA-C	-5.07	1.46	1.52
1	A	560	GLY	N-CA	5.06	1.49	1.45
1	A	519	ILE	C-O	5.06	1.29	1.24
1	A	456	VAL	CA-C	5.03	1.58	1.52
1	C	40	PRO	CA-C	5.01	1.54	1.51
1	B	586	ASN	CA-CB	5.00	1.58	1.53

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	333	VAL	CB-CA-C	-14.86	95.25	111.59
1	A	333	VAL	CB-CA-C	-12.36	94.58	111.63
1	B	333	VAL	CB-CA-C	-11.66	95.54	111.63
1	B	67	VAL	CB-CA-C	-8.32	97.69	110.50
1	B	311	THR	N-CA-CB	-8.32	97.83	110.73
1	C	421	VAL	N-CA-CB	-7.82	100.27	111.21
1	A	474	VAL	N-CA-CB	-7.78	101.62	112.12
1	A	64	MET	CG-SD-CE	-7.75	83.84	100.90
1	B	582	VAL	CB-CA-C	7.71	119.41	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	VAL	N-CA-CB	-7.37	101.37	112.35
1	C	176	SER	CA-C-N	-7.30	113.16	120.31
1	C	176	SER	C-N-CA	-7.30	113.16	120.31
1	B	421	VAL	N-CA-CB	-7.07	101.31	111.21
1	A	578	ARG	NE-CZ-NH2	-7.05	112.85	119.20
1	C	318	GLY	CA-C-N	-6.79	112.23	123.37
1	C	318	GLY	C-N-CA	-6.79	112.23	123.37
1	B	318	GLY	CA-C-N	-6.71	112.69	123.23
1	B	318	GLY	C-N-CA	-6.71	112.69	123.23
1	A	583	ARG	NE-CZ-NH1	6.67	128.17	121.50
1	C	543	THR	N-CA-CB	-6.48	100.33	110.44
1	B	421	VAL	CA-C-N	-6.43	113.10	120.89
1	B	421	VAL	C-N-CA	-6.43	113.10	120.89
1	B	582	VAL	N-CA-CB	-6.35	104.10	112.36
1	B	456	VAL	CG1-CB-CG2	6.25	124.55	110.80
1	A	582	VAL	CG1-CB-CG2	6.22	124.49	110.80
1	B	578	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	B	170	SER	CA-C-N	-6.11	116.27	122.74
1	B	170	SER	C-N-CA	-6.11	116.27	122.74
1	C	451	TYR	CA-C-N	-6.10	114.51	123.05
1	C	451	TYR	C-N-CA	-6.10	114.51	123.05
1	B	609	VAL	CG1-CB-CG2	6.07	124.15	110.80
1	A	162	ALA	N-CA-C	6.00	118.61	111.71
1	B	28	GLU	N-CA-CB	5.74	119.02	109.60
1	C	575	TRP	N-CA-C	5.71	117.50	111.28
1	A	583	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	A	311	THR	CA-CB-CG2	5.66	120.13	110.50
1	C	421	VAL	CG1-CB-CG2	5.66	123.26	110.80
1	C	461	ILE	CA-CB-CG2	5.63	120.07	110.50
1	A	311	THR	N-CA-CB	-5.62	101.71	110.98
1	A	333	VAL	CG1-CB-CG2	5.56	123.04	110.80
1	C	543	THR	OG1-CB-CG2	5.55	120.41	109.30
1	C	578	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	B	617	VAL	CG1-CB-CG2	-5.47	98.77	110.80
1	A	582	VAL	N-CA-CB	-5.46	102.23	111.23
1	C	578	ARG	CB-CG-CD	-5.40	98.89	111.30
1	A	495	THR	N-CA-C	-5.39	106.01	112.59
1	B	318	GLY	N-CA-C	-5.37	104.49	113.02
1	C	543	THR	CA-CB-CG2	5.33	119.57	110.50
1	C	583	ARG	NE-CZ-NH1	5.29	126.78	121.50
1	B	461	ILE	N-CA-CB	-5.28	102.78	111.44
1	C	13	LEU	N-CA-C	-5.27	105.45	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	333	VAL	CG1-CB-CG2	5.26	122.38	110.80
1	A	181	CYS	N-CA-C	5.25	117.42	111.11
1	B	558	ALA	N-CA-C	5.25	117.75	111.71
1	C	617	VAL	CA-C-N	-5.24	114.37	119.76
1	C	617	VAL	C-N-CA	-5.24	114.37	119.76
1	A	474	VAL	CG1-CB-CG2	5.22	122.30	110.80
1	A	456	VAL	CG1-CB-CG2	5.14	122.11	110.80
1	A	578	ARG	CB-CG-CD	-5.08	99.61	111.30
1	A	256	ILE	N-CA-C	5.08	115.73	107.71
1	C	342	ILE	N-CA-C	-5.04	103.16	108.15
1	A	421	VAL	CG1-CB-CG2	5.02	121.85	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	LEU	Peptide
1	A	318	GLY	Peptide
1	C	385	ASN	Mainchain

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	5115	0	5032	89	0
1	B	5120	0	5034	144	1
1	C	5086	0	4992	111	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	24	0	32	2	0
3	B	24	0	31	9	0
3	C	18	0	24	3	0
4	A	10	0	4	0	0
4	C	10	0	4	1	0
5	B	5	0	0	0	0
6	A	1028	0	0	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1051	0	0	45	1
6	C	1116	0	0	46	0
All	All	18610	0	15153	342	2

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 11.

All (342) 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:623:ASP:HB3	6:A:3187:HOH:O	1.15	1.32
1:B:140:MET:HE2	6:B:1901:HOH:O	1.31	1.30
1:C:623:ASP:HB3	6:C:2705:HOH:O	1.20	1.30
1:B:623:ASP:HB3	6:B:1917:HOH:O	1.28	1.28
1:B:43:LYS:HB2	6:B:1590:HOH:O	1.27	1.27
1:C:634:THR:HA	6:C:2441:HOH:O	1.49	1.11
1:B:378:GLN:NE2	1:B:389[B]:MET:CG	2.13	1.11
1:B:351:GLN:HE22	3:B:639:GOL:H11	1.13	1.10
1:B:108:GLU:HG2	1:B:184:LYS:HE2	1.31	1.10
1:B:468:LYS:HE3	1:B:468:LYS:H	1.16	1.08
1:C:468:LYS:H	1:C:468:LYS:CD	1.66	1.08
1:B:378:GLN:HE21	1:B:389[B]:MET:CG	1.67	1.07
1:B:586:ASN:HB2	6:B:812:HOH:O	1.57	1.04
1:A:27:PRO:HD2	6:A:2499:HOH:O	1.56	1.03
1:C:314:SER:HB3	6:C:1988:HOH:O	1.58	1.02
1:C:468:LYS:HD2	1:C:468:LYS:N	1.71	1.02
1:A:124:GLU:HG3	6:A:1791:HOH:O	1.59	1.02
1:C:468:LYS:H	1:C:468:LYS:HD2	0.86	1.01
1:B:378:GLN:NE2	1:B:389[B]:MET:HG3	1.79	0.94
1:B:202:GLU:HG3	6:B:3257:HOH:O	1.66	0.93
1:B:378:GLN:HE21	1:B:389[B]:MET:HG2	1.32	0.93
1:C:403:HIS:HE1	1:C:405:ARG:HE	1.05	0.93
1:A:25:LYS:HE2	6:A:2315:HOH:O	1.68	0.93
1:A:581:ASN:OD1	6:A:3260:HOH:O	1.86	0.93
1:B:2:VAL:HG12	6:B:1378:HOH:O	1.69	0.91
1:B:252:GLU:HG2	6:B:2468:HOH:O	1.70	0.90
1:C:79:LEU:HB2	1:C:89:THR:HG22	1.51	0.90
1:B:448:VAL:H	1:B:453:ASN:HD21	1.10	0.89
1:C:64:MET:SD	6:C:2721:HOH:O	2.31	0.88
1:C:64:MET:CE	6:C:2721:HOH:O	2.22	0.88
1:B:378:GLN:NE2	1:B:389[B]:MET:SD	2.45	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:GLU:CD	1:B:202:GLU:H	1.84	0.86
1:A:43[A]:LYS:HD3	6:A:2602:HOH:O	1.76	0.85
1:A:550:LYS:HE3	6:A:2363:HOH:O	1.73	0.85
1:C:79:LEU:HD13	6:C:896:HOH:O	1.77	0.85
1:B:468:LYS:HE3	1:B:468:LYS:N	1.91	0.84
1:A:318:GLY:HA2	6:A:2462:HOH:O	1.77	0.84
1:B:140:MET:HE3	1:B:140:MET:H	1.43	0.84
1:B:468:LYS:H	1:B:468:LYS:CE	1.92	0.83
1:C:14:GLN:HE21	1:C:339:SER:H	1.26	0.83
1:A:184:LYS:HE3	6:A:1318:HOH:O	1.80	0.82
1:B:468:LYS:HD3	6:B:1087:HOH:O	1.80	0.81
1:B:389[B]:MET:HE3	1:B:391:ASN:OD1	1.81	0.81
1:C:113:ALA:O	1:C:119:VAL:HG11	1.81	0.81
1:A:240:ASN:HB2	6:A:1862:HOH:O	1.81	0.80
1:A:299:GLN:HE22	1:A:535:ASN:HA	1.47	0.79
1:B:28:GLU:HB3	6:B:1372:HOH:O	1.82	0.79
1:C:437:GLN:HE22	1:C:528:LEU:H	1.30	0.79
1:A:437:GLN:HE22	1:A:528:LEU:H	1.31	0.78
1:B:351:GLN:NE2	3:B:639:GOL:H11	1.96	0.78
1:C:144:ASP:OD1	3:C:639:GOL:H31	1.82	0.78
1:B:372:ARG:NH1	1:B:401[B]:ARG:NH1	2.31	0.78
1:C:634:THR:HB	6:C:1080:HOH:O	1.84	0.78
1:B:27:PRO:HD2	6:B:2485:HOH:O	1.83	0.77
1:B:13:LEU:HD21	1:B:333:VAL:HG13	1.65	0.77
1:B:334:ASN:C	1:B:334:ASN:HD22	1.93	0.77
1:C:540:GLN:O	1:C:543:THR:HB	1.83	0.77
1:A:13:LEU:HD21	1:A:333:VAL:HG13	1.66	0.77
1:A:108:GLU:HG2	1:A:184:LYS:HE2	1.65	0.77
1:A:378:GLN:OE1	1:A:389[B]:MET:HG3	1.84	0.77
1:C:403:HIS:CE1	1:C:405:ARG:HE	1.97	0.76
1:C:153:GLN:HE21	1:C:297:ARG:HH22	1.34	0.75
1:C:317:LEU:HD23	6:C:2524:HOH:O	1.85	0.75
3:B:639:GOL:H12	6:B:2035:HOH:O	1.85	0.75
1:B:140:MET:HE1	6:B:1995:HOH:O	1.87	0.74
1:B:116:HIS:HD2	1:B:118:ILE:H	1.32	0.74
1:C:140:MET:SD	6:C:2290:HOH:O	2.46	0.73
1:C:317:LEU:HD21	6:C:2087:HOH:O	1.89	0.73
1:A:378:GLN:OE1	1:A:389[B]:MET:CG	2.36	0.72
1:C:468:LYS:HG3	6:C:2091:HOH:O	1.87	0.72
3:B:639:GOL:H2	6:B:2313:HOH:O	1.88	0.72
3:C:638:GOL:H32	6:C:981:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:VAL:CG1	6:B:1378:HOH:O	2.32	0.71
1:B:577:ARG:HD3	6:B:2040:HOH:O	1.88	0.71
1:B:518:LYS:HE3	1:B:617:VAL:HG11	1.72	0.70
1:B:108:GLU:HG2	1:B:184:LYS:CE	2.17	0.70
1:B:208:GLU:OE1	1:B:417:LYS:HE3	1.92	0.70
1:A:311:THR:HG23	1:A:381:ALA:HB1	1.73	0.70
1:B:35:ILE:HG12	1:B:67:VAL:HG13	1.72	0.70
1:B:111[A]:GLU:HG3	6:B:2658:HOH:O	1.92	0.69
1:A:25:LYS:CE	6:A:2315:HOH:O	2.31	0.69
1:B:311:THR:HG23	1:B:381:ALA:HB1	1.75	0.68
1:C:3:HIS:HD2	1:C:5:TYR:H	1.40	0.68
1:B:311:THR:CG2	1:B:381:ALA:HB1	2.22	0.68
1:A:107[B]:GLN:HG3	6:A:3167:HOH:O	1.93	0.68
1:B:437:GLN:HE22	1:B:528:LEU:H	1.41	0.68
1:C:89:THR:HG23	6:C:640:HOH:O	1.94	0.67
1:B:581:ASN:OD1	6:B:3224:HOH:O	2.11	0.67
1:A:437:GLN:NE2	1:A:528:LEU:H	1.92	0.66
1:C:153:GLN:NE2	1:C:297:ARG:HH12	1.94	0.66
1:C:27:PRO:HD2	6:C:2376:HOH:O	1.96	0.65
1:B:625:ASN:ND2	1:B:627:ALA:H	1.93	0.65
1:A:336[B]:ASN:OD1	6:A:2397:HOH:O	2.15	0.65
1:B:116:HIS:CD2	1:B:118:ILE:H	2.15	0.65
1:C:13:LEU:HD21	1:C:333:VAL:HG13	1.78	0.65
1:B:401[B]:ARG:HD3	6:B:2531:HOH:O	1.97	0.64
1:C:437:GLN:NE2	1:C:528:LEU:H	1.94	0.64
1:C:319:CYS:O	6:C:3253:HOH:O	2.14	0.64
1:B:503:ASN:C	1:B:503:ASN:HD22	2.05	0.64
1:A:311:THR:CG2	1:A:381:ALA:HB1	2.28	0.64
1:C:336:ASN:HB2	6:C:3272:HOH:O	1.97	0.64
1:C:485:LYS:HB2	1:C:486:PRO:HD2	1.80	0.63
1:C:153:GLN:HE22	1:C:297:ARG:HH12	1.44	0.63
1:B:524:ARG:HH12	1:B:612:HIS:CD2	2.16	0.63
1:B:468:LYS:HE2	6:B:2451:HOH:O	1.99	0.63
1:B:372:ARG:NH1	1:B:401[B]:ARG:HH12	1.95	0.63
1:B:399:GLU:OE1	6:B:2531:HOH:O	2.15	0.63
1:C:252:GLU:HG3	6:C:733:HOH:O	1.99	0.63
1:A:95:LYS:HE2	6:A:1863:HOH:O	1.99	0.62
1:B:43:LYS:HE3	1:B:47:ARG:HH12	1.64	0.62
1:A:185:LYS:HE3	6:A:1062:HOH:O	1.99	0.62
1:C:385:ASN:H	1:C:385:ASN:HD22	1.47	0.62
1:C:14:GLN:NE2	1:C:339:SER:H	1.94	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LEU:HB3	6:C:896:HOH:O	1.99	0.62
1:C:385:ASN:H	1:C:385:ASN:ND2	1.97	0.62
1:C:89:THR:HG21	6:C:2488:HOH:O	1.99	0.62
1:C:508:ASN:ND2	1:C:510:ILE:H	1.98	0.62
1:B:351:GLN:HE22	3:B:639:GOL:C1	2.01	0.61
1:B:116:HIS:HE1	4:C:637:TLA:O41	1.83	0.61
1:B:144:ASP:OD2	1:B:296:HIS:HE1	1.83	0.61
1:B:293:ALA:HA	1:B:296:HIS:HD2	1.64	0.61
6:A:2578:HOH:O	1:B:235:GLU:HG2	2.01	0.61
1:B:60:HIS:HB2	6:B:1656:HOH:O	1.99	0.61
1:C:634:THR:HG21	6:C:1895:HOH:O	2.01	0.61
1:C:399:GLU:OE2	6:C:2160:HOH:O	2.16	0.61
1:B:518:LYS:HG3	1:B:617:VAL:HG12	1.81	0.61
1:C:81:ASN:ND2	1:C:84:TYR:H	2.00	0.60
1:B:518:LYS:HE3	1:B:617:VAL:CG1	2.31	0.60
1:A:47:ARG:HD2	6:A:2321:HOH:O	1.99	0.60
1:C:508:ASN:HD22	1:C:510:ILE:H	1.50	0.60
1:B:503:ASN:HD22	1:B:505:ASN:H	1.50	0.60
1:A:586:ASN:HB2	6:A:921:HOH:O	2.01	0.59
1:C:403:HIS:HD2	1:C:613:GLU:OE2	1.85	0.59
1:A:385:ASN:ND2	1:A:385:ASN:H	1.99	0.59
1:A:199:THR:HG22	6:A:2444:HOH:O	2.03	0.59
1:A:241:VAL:HG22	1:A:246:ILE:HD12	1.84	0.59
1:A:378:GLN:OE1	1:A:389[B]:MET:SD	2.61	0.59
1:B:249:GLN:HE21	1:B:396:GLN:HE21	1.50	0.59
1:C:136:CYS:SG	1:C:154:CYS:HB3	2.42	0.59
1:C:503:ASN:HD22	1:C:505:ASN:H	1.51	0.58
1:A:504:GLU:OE2	1:A:583:ARG:HD2	2.03	0.58
1:C:43:LYS:HD3	6:C:1474:HOH:O	2.03	0.58
1:C:184:LYS:HE2	6:C:2476:HOH:O	2.03	0.58
1:C:3:HIS:CD2	1:C:5:TYR:H	2.21	0.58
1:A:43[B]:LYS:HE2	6:A:2322:HOH:O	2.04	0.57
1:B:518:LYS:CG	1:B:617:VAL:HG12	2.34	0.57
1:B:552[A]:ARG:HD3	6:B:1498:HOH:O	2.04	0.57
1:A:503:ASN:HD22	1:A:505:ASN:H	1.50	0.57
1:B:86:HIS:CE1	6:B:3111:HOH:O	2.58	0.57
1:C:468:LYS:HD3	6:C:992:HOH:O	2.04	0.57
1:B:113:ALA:O	1:B:119:VAL:HG11	2.04	0.57
1:B:378:GLN:HE21	1:B:389[B]:MET:HG3	1.50	0.57
1:A:389[A]:MET:HE2	1:B:355:LEU:HD12	1.87	0.56
1:B:399:GLU:CD	1:B:401[B]:ARG:HH11	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:LYS:HD3	6:C:2560:HOH:O	2.06	0.56
1:C:485:LYS:HA	1:C:582:VAL:HG22	1.87	0.56
1:B:625:ASN:HD22	1:B:627:ALA:H	1.54	0.55
1:B:526:MET:H	3:B:640:GOL:C1	2.18	0.55
1:A:184:LYS:HD3	6:A:2311:HOH:O	2.06	0.55
1:C:485:LYS:HB2	1:C:486:PRO:CD	2.36	0.55
1:C:219:ASN:C	1:C:219:ASN:HD22	2.15	0.55
1:C:504:GLU:OE2	1:C:583:ARG:HD2	2.07	0.55
1:C:581[A]:ASN:ND2	1:C:583:ARG:H	2.05	0.55
1:A:230:ILE:CG2	6:B:2064:HOH:O	2.55	0.55
1:C:115:THR:HG22	6:C:1410:HOH:O	2.07	0.55
1:B:249:GLN:NE2	1:B:396:GLN:HE21	2.06	0.54
1:B:437:GLN:NE2	1:B:528:LEU:H	2.04	0.54
1:B:534:TYR:O	1:B:538:ARG:HG3	2.07	0.54
1:C:399:GLU:OE1	1:C:401:ARG:HD2	2.06	0.54
1:A:578:ARG:HD2	1:A:580:GLU:OE2	2.07	0.54
1:B:383:VAL:O	1:B:386:TPQ:H6	2.07	0.53
1:A:399:GLU:OE1	1:A:401:ARG:HD2	2.08	0.53
1:B:597:HIS:O	1:B:599:PRO:HD3	2.08	0.53
1:C:64:MET:HE2	6:C:2721:HOH:O	2.02	0.53
1:B:275:VAL:HG12	1:B:276:VAL:HG23	1.90	0.53
1:C:47:ARG:HD2	6:C:2310:HOH:O	2.09	0.53
1:B:293:ALA:HA	1:B:296:HIS:CD2	2.45	0.52
1:B:526:MET:H	3:B:640:GOL:H12	1.75	0.52
1:C:208:GLU:HB3	6:C:2643:HOH:O	2.09	0.52
1:A:421:VAL:HG22	1:A:423:TRP:CZ2	2.44	0.52
1:B:625:ASN:HD22	1:B:625:ASN:C	2.18	0.52
1:C:383:VAL:O	1:C:386:TPQ:H6	2.10	0.52
1:A:385:ASN:H	1:A:385:ASN:HD22	1.57	0.52
1:B:108:GLU:CG	1:B:184:LYS:HE2	2.22	0.52
1:B:634:THR:C	6:B:2011:HOH:O	2.53	0.52
1:C:604:PHE:CG	1:C:605:PRO:HA	2.45	0.52
1:C:31:HIS:HD2	6:C:1564:HOH:O	1.93	0.51
3:A:639:GOL:H11	6:A:2301:HOH:O	2.11	0.51
1:B:184:LYS:HD2	6:B:2433:HOH:O	2.10	0.51
1:C:81:ASN:C	1:C:81:ASN:HD22	2.19	0.51
1:B:399:GLU:CD	1:B:401[B]:ARG:NH1	2.69	0.51
1:A:503:ASN:HD22	1:A:503:ASN:C	2.18	0.51
1:B:240:ASN:HB2	6:B:1111:HOH:O	2.11	0.51
1:C:251:TRP:C	1:C:252:GLU:HG2	2.35	0.51
1:A:226:LEU:HD22	1:B:373:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ARG:HD2	1:B:580:GLU:OE2	2.11	0.51
1:B:524:ARG:HH12	1:B:612:HIS:HD2	1.56	0.50
1:C:568:THR:HG22	6:C:2535:HOH:O	2.09	0.50
1:A:504:GLU:OE2	1:A:583:ARG:CD	2.59	0.50
1:A:230:ILE:HG21	6:B:2064:HOH:O	2.12	0.50
1:C:503:ASN:HD22	1:C:503:ASN:C	2.19	0.50
1:C:144:ASP:OD1	3:C:639:GOL:C3	2.58	0.50
1:B:101:LEU:HG	1:B:106:ILE:HD11	1.94	0.49
1:B:334:ASN:C	1:B:334:ASN:ND2	2.65	0.49
1:C:578:ARG:HD2	1:C:580:GLU:OE2	2.10	0.49
1:A:307:GLY:O	1:A:311:THR:HB	2.12	0.49
1:C:31:HIS:HE1	1:C:105:ASP:OD2	1.94	0.49
1:A:230:ILE:HB	6:B:2064:HOH:O	2.11	0.49
1:C:219:ASN:HD22	1:C:221:GLU:H	1.60	0.49
1:C:403:HIS:HE1	1:C:405:ARG:NE	1.89	0.49
1:A:389[B]:MET:HE1	1:B:355:LEU:HB2	1.95	0.49
1:C:219:ASN:ND2	1:C:221:GLU:H	2.11	0.49
1:C:399:GLU:OE1	1:C:401:ARG:CD	2.61	0.49
1:A:435:TYR:HB3	1:B:476:PHE:CE2	2.48	0.48
1:B:405:ARG:HB3	1:B:609:VAL:HG22	1.96	0.48
1:C:503:ASN:HD21	1:C:505:ASN:HD22	1.62	0.48
1:B:555:GLU:CD	1:B:578:ARG:HH22	2.21	0.48
1:A:185:LYS:HB3	1:A:185:LYS:HE2	1.57	0.48
1:B:625:ASN:HD22	1:B:626:PRO:N	2.11	0.48
1:C:437:GLN:HE22	1:C:528:LEU:N	2.04	0.48
1:A:239:PHE:CE1	1:A:326:LYS:HG3	2.49	0.48
1:B:16:THR:CG2	1:B:67:VAL:HG22	2.44	0.48
1:C:338:ASP:OD1	6:C:3025:HOH:O	2.20	0.48
1:B:208:GLU:CD	1:B:417:LYS:HE3	2.38	0.47
1:B:524:ARG:HH22	1:B:612:HIS:HD2	1.63	0.47
1:C:380:ILE:HG12	1:C:389:MET:HG2	1.96	0.47
1:B:307:GLY:O	1:B:311:THR:HB	2.14	0.47
1:C:318:GLY:HA3	6:C:2293:HOH:O	2.13	0.47
1:C:326:LYS:HE3	6:C:2477:HOH:O	2.13	0.47
1:B:185:LYS:NZ	6:B:1462:HOH:O	2.47	0.47
1:B:417:LYS:HE2	6:B:1082:HOH:O	2.14	0.47
1:C:131:HIS:H	1:C:131:HIS:CD2	2.33	0.47
1:C:426:ASN:ND2	6:C:962:HOH:O	2.47	0.47
1:A:462:ARG:NH1	1:B:529:ALA:O	2.48	0.47
1:A:437:GLN:HE22	1:A:528:LEU:N	2.06	0.47
1:A:389[B]:MET:HG2	1:A:391:ASN:HD21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LYS:HE3	1:A:579:ASP:OD2	2.16	0.46
1:A:531:GLU:HG2	6:B:2593:HOH:O	2.15	0.46
1:B:372:ARG:HH11	1:B:401[B]:ARG:HH12	1.61	0.46
1:B:401[A]:ARG:HD2	6:B:2531:HOH:O	2.15	0.46
1:A:568:THR:HG22	6:A:1048:HOH:O	2.15	0.46
1:A:273:ARG:HD3	6:A:1045:HOH:O	2.15	0.46
1:B:391:ASN:ND2	3:B:639:GOL:O3	2.49	0.46
1:B:503:ASN:ND2	1:B:505:ASN:H	2.13	0.46
1:C:31:HIS:CD2	6:C:1564:HOH:O	2.69	0.46
1:A:284:MET:HE1	1:A:388:TYR:CE1	2.51	0.45
1:C:550:LYS:HE2	6:C:2960:HOH:O	2.17	0.45
1:A:634:THR:C	6:A:930:HOH:O	2.59	0.45
1:B:426:ASN:ND2	6:B:1003:HOH:O	2.48	0.45
1:B:468:LYS:H	1:B:468:LYS:CD	2.28	0.45
1:A:417:LYS:CD	6:A:2257:HOH:O	2.64	0.45
1:B:314[A]:SER:OG	6:B:1311:HOH:O	2.20	0.45
1:A:299:GLN:NE2	1:A:535:ASN:HA	2.23	0.45
1:B:552[B]:ARG:NH2	1:B:580:GLU:OE1	2.43	0.45
1:A:399:GLU:OE1	1:A:401:ARG:CD	2.65	0.45
1:B:456:VAL:HG12	1:B:500:LYS:HB2	1.99	0.45
3:A:639:GOL:O3	6:A:2614:HOH:O	2.20	0.44
1:B:417:LYS:HD2	1:B:430:ARG:HD3	1.99	0.44
1:C:253:PHE:HB3	1:C:268:ILE:HA	2.00	0.44
1:A:242:ASP:HB2	6:A:2572:HOH:O	2.16	0.44
1:B:302:ASP:O	1:B:306[B]:CYS:HB2	2.18	0.44
1:A:108:GLU:HG2	1:A:184:LYS:CE	2.41	0.44
1:C:437:GLN:HE22	1:C:527:LEU:HA	1.82	0.44
1:B:585:ASP:CB	6:B:1852:HOH:O	2.66	0.44
1:B:140:MET:CE	6:B:1901:HOH:O	2.16	0.44
1:A:286:VAL:HA	1:A:437:GLN:O	2.18	0.44
1:B:110:GLU:HB2	1:B:138:PRO:HG2	2.00	0.44
1:B:503:ASN:HD21	1:B:505:ASN:HD22	1.64	0.44
1:B:111[A]:GLU:CG	6:B:2658:HOH:O	2.59	0.44
1:B:604:PHE:CG	1:B:605:PRO:HA	2.52	0.44
1:C:25:LYS:HA	6:C:3005:HOH:O	2.17	0.44
1:C:299:GLN:OE1	1:C:535:ASN:HA	2.18	0.43
1:C:543:THR:HG22	1:C:547:TRP:HZ2	1.82	0.43
1:C:555:GLU:OE2	1:C:578:ARG:NH2	2.39	0.43
1:A:53:ARG:HG3	6:A:1822:HOH:O	2.17	0.43
1:B:376:VAL:CG1	1:B:391:ASN:HD22	2.31	0.43
1:A:604:PHE:CG	1:A:605:PRO:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:THR:HG23	6:C:860:HOH:O	2.17	0.43
1:A:383:VAL:O	1:A:386:TPQ:H6	2.17	0.43
1:B:389[A]:MET:HE3	1:B:407:THR:HG21	2.00	0.43
1:A:67:VAL:CG1	1:A:78:ALA:HB3	2.49	0.43
1:A:158:LEU:HD22	1:A:173:LEU:HD21	2.01	0.43
1:C:537:LYS:HD3	1:C:537:LYS:HA	1.84	0.42
1:A:633:SER:O	1:A:634:THR:C	2.62	0.42
1:B:448:VAL:H	1:B:453:ASN:ND2	1.94	0.42
1:B:502:ILE:HG22	1:B:516:ALA:HB2	2.01	0.42
1:B:568:THR:HG22	6:B:1038:HOH:O	2.19	0.42
1:B:33:ILE:HG22	1:B:100:PRO:HG2	2.01	0.42
1:B:288:TYR:OH	1:B:386:TPQ:O4	2.18	0.42
1:B:547:TRP:HB2	1:B:590:TRP:HB2	2.00	0.42
1:C:537:LYS:CE	6:C:2382:HOH:O	2.66	0.42
1:C:537:LYS:HE3	6:C:2382:HOH:O	2.19	0.42
1:A:232:GLN:HE21	1:A:232:GLN:HB2	1.58	0.42
1:C:333:VAL:HG12	1:C:337:GLY:HA2	2.01	0.42
1:A:204:GLN:HG2	6:A:1713:HOH:O	2.19	0.42
1:A:491:GLN:OE1	1:A:523:ALA:HA	2.19	0.42
1:B:526:MET:N	3:B:640:GOL:H12	2.35	0.42
1:C:503:ASN:ND2	1:C:505:ASN:HD22	2.17	0.42
1:A:407:THR:HA	1:A:607:MET:HG3	2.01	0.42
1:A:472:TYR:CE2	1:B:144:ASP:HB2	2.55	0.42
1:B:518:LYS:CE	1:B:617:VAL:CG1	2.98	0.42
1:C:410:LEU:HD13	1:C:433:ALA:CB	2.50	0.42
1:A:136:CYS:SG	1:A:154:CYS:HB3	2.60	0.42
1:C:108:GLU:HG2	1:C:184:LYS:HD3	2.01	0.42
1:A:43[A]:LYS:HE2	6:A:2474:HOH:O	2.19	0.42
1:A:289:GLY:O	1:B:475:GLY:HA2	2.20	0.42
1:A:555:GLU:CD	1:A:578:ARG:HH22	2.25	0.42
6:A:1826:HOH:O	1:B:227:LYS:HE3	2.18	0.41
1:C:158:LEU:HD13	1:C:173:LEU:HD11	2.02	0.41
1:A:56:LYS:HG3	6:A:2654:HOH:O	2.20	0.41
1:A:285:THR:HA	1:A:300:ALA:O	2.20	0.41
1:B:470:ASN:HD21	1:B:475:GLY:H	1.67	0.41
1:C:259:VAL:HG21	6:C:886:HOH:O	2.20	0.41
1:A:170:SER:CB	1:A:212:VAL:H	2.34	0.41
1:C:167:ASN:HD21	1:C:169:TYR:HB2	1.85	0.41
1:C:288:TYR:CD2	1:C:436:HIS:HB3	2.56	0.41
1:B:597:HIS:CD2	1:B:597:HIS:C	2.98	0.41
1:C:79:LEU:HB2	1:C:89:THR:CG2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:LEU:N	1:C:440:LEU:HD12	2.35	0.41
1:A:407:THR:HA	1:A:607:MET:CG	2.50	0.41
1:B:117:PRO:HG3	6:C:1599:HOH:O	2.20	0.41
1:C:50:GLU:OE2	1:C:53:ARG:NH1	2.54	0.41
1:B:299:GLN:OE1	1:B:535:ASN:HA	2.20	0.41
1:B:468:LYS:HG2	6:B:1395:HOH:O	2.21	0.41
1:C:219:ASN:HD22	1:C:220:GLY:N	2.18	0.41
1:B:111[A]:GLU:CD	6:B:2658:HOH:O	2.64	0.41
1:B:131:HIS:HD2	6:B:2296:HOH:O	2.04	0.41
1:C:543:THR:CG2	6:C:860:HOH:O	2.69	0.41
1:B:492:SER:HB3	1:B:497:ARG:HB2	2.03	0.40
1:C:378:GLN:NE2	6:C:2679:HOH:O	2.46	0.40
1:A:204:GLN:CG	6:A:1713:HOH:O	2.69	0.40
1:A:308:PHE:HA	1:A:311:THR:HG22	2.03	0.40
1:A:372:ARG:NH2	6:A:1497:HOH:O	2.54	0.40
1:B:532:ASP:OD2	6:B:2724:HOH:O	2.22	0.40
1:B:135:VAL:HG22	1:B:168:HIS:CD2	2.56	0.40
1:B:444:ILE:O	1:B:446:PRO:HD3	2.21	0.40
1:C:2:VAL:HG21	6:C:2786:HOH:O	2.21	0.40
1:A:317:LEU:CD2	6:A:1061:HOH:O	2.70	0.40
1:B:367:PRO:HG3	6:B:2068:HOH:O	2.21	0.40
1:B:468:LYS:CG	6:B:1395:HOH:O	2.69	0.40
1:B:593:LEU:HD21	1:B:612:HIS:HB3	2.03	0.40

All (2) 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:B:84:TYR:OH	1:B:86:HIS:NE2[2_556]	2.02	0.18
6:B:1986:HOH:O	6:B:2006:HOH:O[2_556]	2.17	0.03

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	636/633 (100%)	618 (97%)	17 (3%)	1 (0%)	43	42
1	B	636/633 (100%)	619 (97%)	17 (3%)	0	100	100
1	C	631/633 (100%)	613 (97%)	18 (3%)	0	100	100
All	All	1903/1899 (100%)	1850 (97%)	52 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	LEU

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	563/558 (101%)	539 (96%)	24 (4%)	26	25
1	B	563/558 (101%)	532 (94%)	31 (6%)	19	17
1	C	558/558 (100%)	532 (95%)	26 (5%)	23	22
All	All	1684/1674 (101%)	1603 (95%)	81 (5%)	23	21

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

Mol	Chain	Res	Type
1	A	53	ARG
1	A	95	LYS
1	A	108	GLU
1	A	158	LEU
1	A	226	LEU
1	A	238	SER
1	A	273	ARG
1	A	311	THR
1	A	326	LYS
1	A	333	VAL

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Mol	Chain	Res	Type
1	A	355	LEU
1	A	385	ASN
1	A	421	VAL
1	A	456	VAL
1	A	474	VAL
1	A	485	LYS
1	A	486	PRO
1	A	503	ASN
1	A	536	ASN
1	A	577	ARG
1	A	582	VAL
1	A	583	ARG
1	A	624	LYS
1	A	628	LEU
1	B	28	GLU
1	B	37	ARG
1	B	43	LYS
1	B	53	ARG
1	B	79	LEU
1	B	101	LEU
1	B	108	GLU
1	B	115	THR
1	B	120	LYS
1	B	135	VAL
1	B	140	MET
1	B	146	LYS
1	B	158	LEU
1	B	184	LYS
1	B	202	GLU
1	B	226	LEU
1	B	227	LYS
1	B	238	SER
1	B	246	ILE
1	B	311	THR
1	B	317	LEU
1	B	333	VAL
1	B	334	ASN
1	B	417	LYS
1	B	421	VAL
1	B	456	VAL
1	B	461	ILE
1	B	468	LYS

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Mol	Chain	Res	Type
1	B	503	ASN
1	B	582	VAL
1	B	617	VAL
1	C	20	ILE
1	C	79	LEU
1	C	81	ASN
1	C	89	THR
1	C	108	GLU
1	C	146	LYS
1	C	158	LEU
1	C	219	ASN
1	C	230	ILE
1	C	246	ILE
1	C	252	GLU
1	C	308	PHE
1	C	326	LYS
1	C	333	VAL
1	C	385	ASN
1	C	421	VAL
1	C	461	ILE
1	C	468	LYS
1	C	485	LYS
1	C	503	ASN
1	C	508	ASN
1	C	543	THR
1	C	581[A]	ASN
1	C	581[B]	ASN
1	C	583	ARG
1	C	634	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	232	GLN
1	A	240	ASN
1	A	299	GLN
1	A	344	ASN
1	A	385	ASN
1	A	437	GLN
1	A	503	ASN
1	A	525	GLN

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Mol	Chain	Res	Type
1	A	545	GLN
1	B	90	ASN
1	B	116	HIS
1	B	167	ASN
1	B	204	GLN
1	B	296	HIS
1	B	334	ASN
1	B	351	GLN
1	B	378	GLN
1	B	391	ASN
1	B	396	GLN
1	B	426	ASN
1	B	437	GLN
1	B	453	ASN
1	B	466	ASN
1	B	470	ASN
1	B	503	ASN
1	B	536	ASN
1	B	540	GLN
1	B	545	GLN
1	B	612	HIS
1	B	625	ASN
1	C	3	HIS
1	C	14	GLN
1	C	18	GLN
1	C	31	HIS
1	C	81	ASN
1	C	131	HIS
1	C	141	ASN
1	C	153	GLN
1	C	167	ASN
1	C	168	HIS
1	C	219	ASN
1	C	232	GLN
1	C	244	HIS
1	C	351	GLN
1	C	378	GLN
1	C	385	ASN
1	C	391	ASN
1	C	403	HIS
1	C	426	ASN
1	C	437	GLN

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Mol	Chain	Res	Type
1	C	503	ASN
1	C	508	ASN
1	C	525	GLN
1	C	567	GLN

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
1	TPQ	B	386	1	13,14,15	1.91	6 (46%)	13,19,21	1.43	3 (23%)
1	TPQ	A	386	1	13,14,15	2.40	6 (46%)	13,19,21	1.40	1 (7%)
1	TPQ	C	386	1	13,14,15	1.55	4 (30%)	13,19,21	1.40	2 (15%)

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	TPQ	B	386	1	-	0/5/22/24	0/1/1/1
1	TPQ	A	386	1	-	0/5/22/24	0/1/1/1
1	TPQ	C	386	1	-	0/5/22/24	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	TPQ	O2-C2	4.20	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	TPQ	O5-C5	4.06	1.35	1.24
1	A	386	TPQ	C3-C4	3.14	1.41	1.36
1	B	386	TPQ	O5-C5	3.10	1.32	1.24
1	A	386	TPQ	CB-CA	-2.99	1.47	1.53
1	B	386	TPQ	C6-C5	-2.99	1.36	1.44
1	C	386	TPQ	O5-C5	2.92	1.32	1.24
1	A	386	TPQ	C3-C2	-2.80	1.37	1.44
1	B	386	TPQ	C3-C2	-2.46	1.38	1.44
1	B	386	TPQ	O2-C2	2.41	1.31	1.24
1	A	386	TPQ	C6-C1	2.38	1.40	1.34
1	B	386	TPQ	C1-C2	-2.37	1.45	1.49
1	B	386	TPQ	CB-CA	-2.34	1.48	1.53
1	C	386	TPQ	O2-C2	2.19	1.30	1.24
1	C	386	TPQ	C6-C5	-2.18	1.39	1.44
1	C	386	TPQ	C3-C2	-2.16	1.39	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	TPQ	C6-C1-C2	3.52	121.16	118.66
1	C	386	TPQ	C6-C5-C4	2.74	121.59	116.80
1	B	386	TPQ	O2-C2-C1	-2.61	115.74	120.96
1	C	386	TPQ	C3-C4-C5	-2.44	118.74	121.23
1	B	386	TPQ	C3-C4-C5	-2.36	118.83	121.23
1	B	386	TPQ	C6-C5-C4	2.12	120.52	116.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	386	TPQ	2	0
1	A	386	TPQ	1	0
1	C	386	TPQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	636	-	5,5,5	1.10	0	5,5,5	0.90	0
3	GOL	B	637	-	5,5,5	0.43	0	5,5,5	0.80	0
3	GOL	A	639	-	5,5,5	0.49	0	5,5,5	1.03	1 (20%)
3	GOL	A	636	-	5,5,5	0.48	0	5,5,5	1.40	1 (20%)
3	GOL	C	636	-	5,5,5	1.02	0	5,5,5	0.98	0
3	GOL	B	639	-	5,5,5	0.66	0	5,5,5	1.20	0
3	GOL	A	638	-	5,5,5	1.08	0	5,5,5	1.11	1 (20%)
3	GOL	C	638	-	5,5,5	0.58	0	5,5,5	1.11	0
3	GOL	A	637	-	5,5,5	0.37	0	5,5,5	2.08	2 (40%)
3	GOL	C	639	-	5,5,5	0.39	0	5,5,5	0.85	0
5	PO4	B	638	-	4,4,4	0.95	0	6,6,6	0.64	0
4	TLA	C	637	-	9,9,9	1.93	3 (33%)	12,12,12	1.67	3 (25%)
3	GOL	B	640	-	5,5,5	0.34	0	5,5,5	1.06	0
4	TLA	A	640	-	9,9,9	1.77	3 (33%)	12,12,12	1.52	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
3	GOL	B	636	-	-	1/4/4/4	-
3	GOL	B	637	-	-	0/4/4/4	-
3	GOL	A	639	-	-	0/4/4/4	-
3	GOL	A	636	-	-	2/4/4/4	-
3	GOL	C	636	-	-	2/4/4/4	-
3	GOL	B	639	-	-	2/4/4/4	-
3	GOL	A	638	-	-	0/4/4/4	-
3	GOL	C	638	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	637	-	-	4/4/4/4	-
3	GOL	C	639	-	-	0/4/4/4	-
4	TLA	C	637	-	-	0/12/12/12	-
3	GOL	B	640	-	-	3/4/4/4	-
4	TLA	A	640	-	-	0/12/12/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	637	TLA	C3-C4	-4.20	1.46	1.52
4	A	640	TLA	O2-C2	2.49	1.47	1.42
4	A	640	TLA	C2-C1	-2.23	1.49	1.52
4	C	637	TLA	O1-C1	2.19	1.28	1.22
4	C	637	TLA	C2-C1	-2.17	1.49	1.52
4	A	640	TLA	O11-C1	-2.13	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	640	TLA	O41-C4-C3	3.36	122.66	113.31
4	C	637	TLA	O3-C3-C4	-3.17	103.92	110.69
3	A	637	GOL	O3-C3-C2	-3.16	96.17	110.38
3	A	637	GOL	O2-C2-C1	2.99	121.55	109.18
4	C	637	TLA	O1-C1-C2	-2.86	114.01	121.62
3	A	636	GOL	C3-C2-C1	-2.59	102.31	111.80
4	C	637	TLA	O11-C1-C2	2.34	119.82	113.31
3	A	639	GOL	C3-C2-C1	-2.18	103.82	111.80
3	A	638	GOL	O3-C3-C2	2.10	119.84	110.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	636	GOL	C1-C2-C3-O3
3	A	637	GOL	O1-C1-C2-C3
3	A	637	GOL	C1-C2-C3-O3
3	B	640	GOL	C1-C2-C3-O3
3	C	636	GOL	O1-C1-C2-C3
3	C	638	GOL	O1-C1-C2-C3
3	C	638	GOL	C1-C2-C3-O3
3	A	637	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	639	GOL	O1-C1-C2-C3
3	A	636	GOL	O2-C2-C3-O3
3	A	637	GOL	O2-C2-C3-O3
3	C	638	GOL	O2-C2-C3-O3
3	C	636	GOL	O1-C1-C2-O2
3	B	640	GOL	O1-C1-C2-C3
3	B	639	GOL	O1-C1-C2-O2
3	B	640	GOL	O2-C2-C3-O3
3	C	638	GOL	O1-C1-C2-O2
3	B	636	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	639	GOL	2	0
3	B	639	GOL	6	0
3	C	638	GOL	1	0
3	C	639	GOL	2	0
4	C	637	TLA	1	0
3	B	640	GOL	3	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 [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	632/633 (99%)	-0.80	2 (0%) 90 89	13, 24, 38, 59	6 (0%)
1	B	632/633 (99%)	-0.69	6 (0%) 81 80	11, 25, 40, 62	6 (0%)
1	C	632/633 (99%)	-0.83	1 (0%) 91 90	15, 22, 36, 57	1 (0%)
All	All	1896/1899 (99%)	-0.78	9 (0%) 87 87	11, 24, 39, 62	13 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	LEU	4.3
1	C	318	GLY	3.0
1	A	318	GLY	2.9
1	B	319	CYS	2.4
1	B	597	HIS	2.2
1	B	84	TYR	2.1
1	A	317	LEU	2.1
1	B	318	GLY	2.1
1	B	202	GLU	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
1	TPQ	B	386	14/15	0.96	0.07	18,24,27,28	1
1	TPQ	C	386	14/15	0.96	0.06	16,22,29,29	1
1	TPQ	A	386	14/15	0.98	0.05	18,26,29,29	1

6.3 Carbohydrates ⓘ

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
5	PO4	B	638	5/5	0.85	0.22	125,125,126,126	0
3	GOL	B	640	6/6	0.86	0.17	40,52,54,60	0
3	GOL	B	639	6/6	0.91	0.13	48,56,57,57	0
3	GOL	C	639	6/6	0.92	0.11	53,54,57,58	0
3	GOL	A	636	6/6	0.93	0.13	49,53,56,56	0
3	GOL	A	637	6/6	0.93	0.11	35,41,44,45	0
3	GOL	A	639	6/6	0.93	0.10	39,43,46,51	0
3	GOL	B	636	6/6	0.93	0.09	20,26,31,31	0
3	GOL	C	638	6/6	0.94	0.12	41,51,57,58	0
3	GOL	A	638	6/6	0.95	0.08	21,27,29,30	0
3	GOL	B	637	6/6	0.95	0.09	41,42,45,47	0
3	GOL	C	636	6/6	0.95	0.08	21,30,31,31	0
4	TLA	A	640	10/10	0.97	0.05	21,25,28,28	0
4	TLA	C	637	10/10	0.98	0.04	24,27,30,30	0
2	CU	B	635	1/1	0.99	0.02	24,24,24,24	0
2	CU	A	635	1/1	1.00	0.01	22,22,22,22	0
2	CU	C	635	1/1	1.00	0.01	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.