



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 05:09 AM EDT

PDB ID : 2RDB  
Title : X-ray Crystal Structure of Toluene/o-Xylene Monooxygenase Hydroxylase I100W Mutant  
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Deposited on : 2007-09-21  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

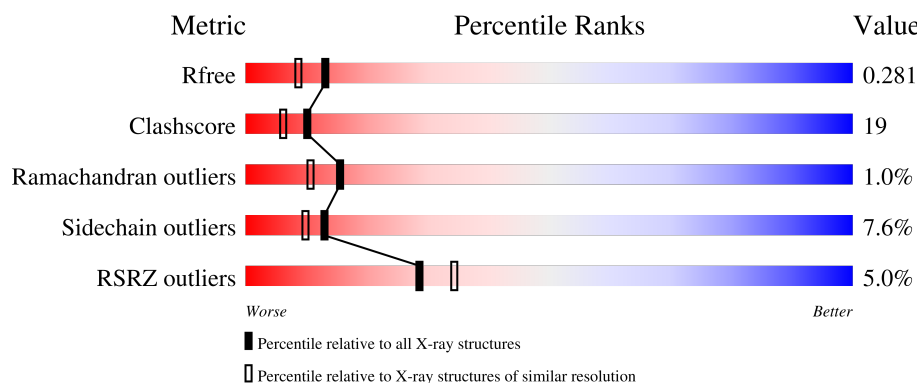
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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  $\geq 3$ , 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	498	<div> <div>5%</div> <div>57%</div> <div>35%</div> <div>6%</div> <div>..</div> </div>
2	B	330	<div> <div>5%</div> <div>61%</div> <div>30%</div> <div>7%</div> <div>.</div> </div>
3	C	86	<div> <div>3%</div> <div>35%</div> <div>47%</div> <div>12%</div> <div>..</div> </div>

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
5	P6G	A	4974	-	-	X	-
7	MPO	B	4401	-	X	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7556 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 Toluene, o-xylene monooxygenase oxygenase subunit;alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	1	0
			4035	2580	676	753	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	TRP	ILE	engineered mutation	UNP O87798

- Molecule 2 is a protein called Toluene, o-xylene monooxygenase oxygenase subunit;beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	0	0
			2641	1674	467	490	10			

- Molecule 3 is a protein called Toluene, o-xylene monooxygenase oxygenase subunit;gamma.

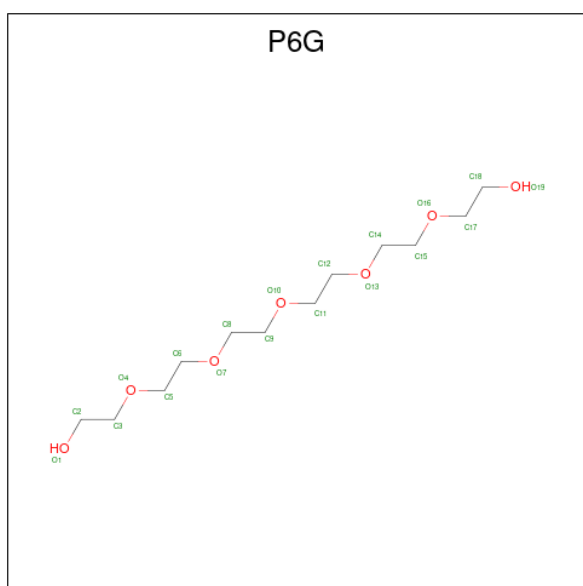
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	83	Total	C	N	O	S	0	0	0
			676	425	120	126	5			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).

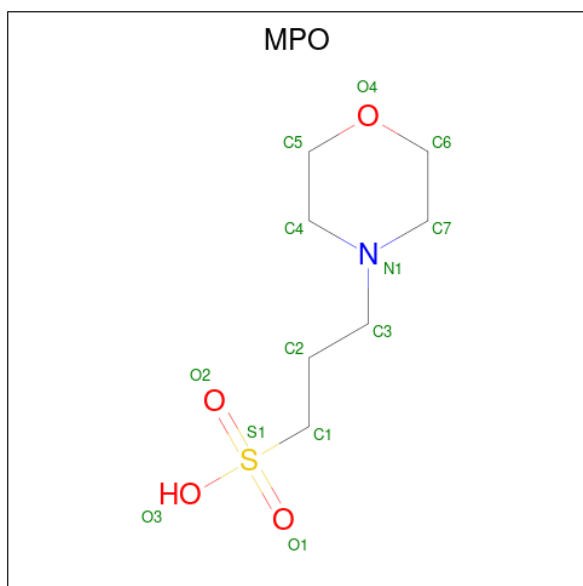


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Fe	0	0
			2	2		

- Molecule 7 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

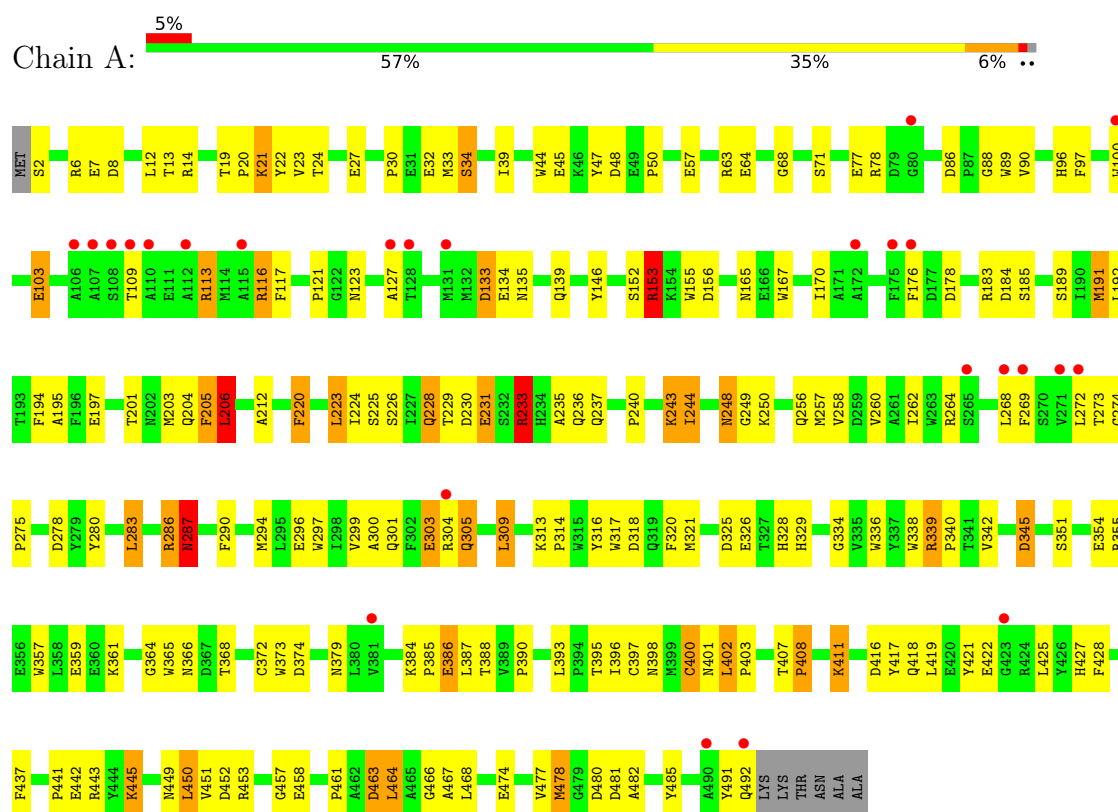
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	82	Total	O	0	0
			82	82		
8	B	72	Total	O	0	0
			72	72		
8	C	4	Total	O	0	0
			4	4		

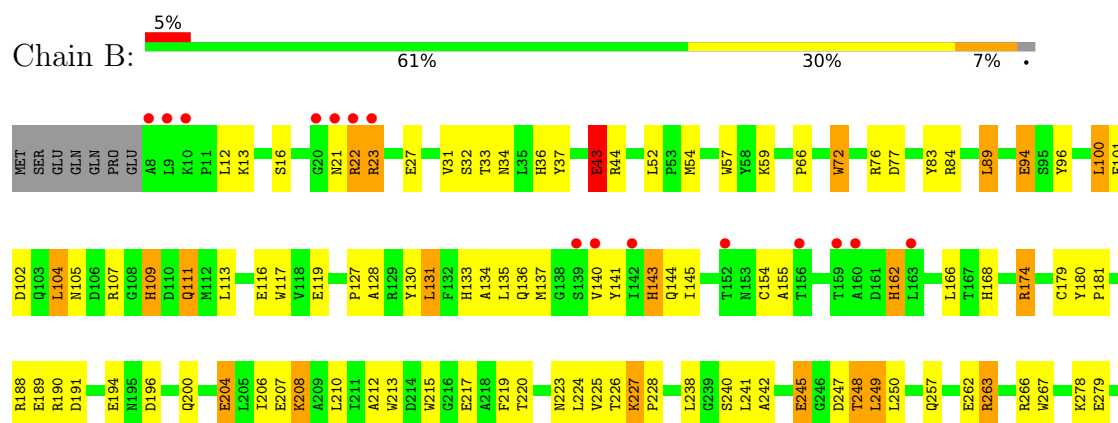
### 3 Residue-property plots

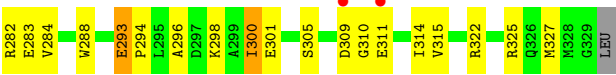
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Toluene, o-xylene monooxygenase oxygenase subunit;alpha



- Molecule 2: Toluene, o-xylene monooxygenase oxygenase subunit;beta





● Molecule 3: Toluene, o-xylene monooxygenase oxygenase subunit;gamma





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.42Å 182.42Å 67.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.84 – 2.10 36.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	84.7 (36.84-2.10) 84.4 (36.83-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.48 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.217 , 0.284 0.218 , 0.281	Depositor DCC
$R_{free}$ test set	3687 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.952	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7556	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, P6G, FE, MPO

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	1.61	29/4166 (0.7%)	1.34	32/5664 (0.6%)
2	B	1.69	27/2713 (1.0%)	1.43	27/3688 (0.7%)
3	C	1.45	2/690 (0.3%)	1.42	7/934 (0.7%)
All	All	1.63	58/7569 (0.8%)	1.38	66/10286 (0.6%)

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

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	TYR	CD1-CE1	13.31	1.59	1.39
1	A	64	GLU	CB-CG	10.37	1.71	1.52
2	B	43	GLU	CG-CD	10.24	1.67	1.51
2	B	283	GLU	CG-CD	10.23	1.67	1.51
1	A	146	TYR	CD1-CE1	-9.87	1.24	1.39
2	B	262	GLU	CG-CD	8.20	1.64	1.51
1	A	97	PHE	CG-CD2	7.84	1.50	1.38
1	A	437	PHE	CD2-CE2	7.83	1.54	1.39
2	B	43	GLU	CB-CG	7.79	1.67	1.52
1	A	7	GLU	CG-CD	7.45	1.63	1.51
1	A	57	GLU	CG-CD	7.40	1.63	1.51
3	C	32	GLU	CG-CD	7.17	1.62	1.51
2	B	219	PHE	CE1-CZ	7.14	1.50	1.37
2	B	325	ARG	CZ-NH2	7.06	1.42	1.33
2	B	131	LEU	C-O	-7.05	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	135	LEU	N-CA	7.04	1.60	1.46
1	A	103	GLU	CB-CG	6.91	1.65	1.52
1	A	231	GLU	CD-OE2	6.91	1.33	1.25
1	A	457	GLY	N-CA	-6.59	1.36	1.46
2	B	283	GLU	CB-CG	6.59	1.64	1.52
1	A	231	GLU	CB-CG	6.55	1.64	1.52
1	A	194	PHE	CD1-CE1	6.50	1.52	1.39
1	A	64	GLU	CG-CD	6.29	1.61	1.51
1	A	189	SER	CB-OG	6.23	1.50	1.42
2	B	72	TRP	CZ3-CH2	6.12	1.49	1.40
1	A	374	ASP	N-CA	6.11	1.58	1.46
2	B	301	GLU	CD-OE1	6.11	1.32	1.25
1	A	458	GLU	CB-CG	6.06	1.63	1.52
2	B	107	ARG	CZ-NH2	5.85	1.40	1.33
1	A	442	GLU	CD-OE2	5.84	1.32	1.25
2	B	94	GLU	CD-OE1	5.81	1.32	1.25
2	B	37	TYR	CB-CG	5.79	1.60	1.51
2	B	217	GLU	CD-OE2	-5.59	1.19	1.25
2	B	213	TRP	CB-CG	5.57	1.60	1.50
1	A	117	PHE	CA-CB	5.54	1.66	1.53
2	B	212	ALA	CA-CB	5.54	1.64	1.52
1	A	205	PHE	CE2-CZ	5.46	1.47	1.37
2	B	130	TYR	CD1-CE1	5.46	1.47	1.39
1	A	45	GLU	CD-OE1	5.44	1.31	1.25
1	A	113	ARG	CB-CG	5.41	1.67	1.52
2	B	300	ILE	CA-CB	5.39	1.67	1.54
2	B	101	PHE	CD1-CE1	-5.29	1.28	1.39
1	A	342	VAL	CB-CG1	5.28	1.64	1.52
1	A	464	LEU	CG-CD1	5.26	1.71	1.51
2	B	245	GLU	CD-OE2	5.26	1.31	1.25
1	A	400	CYS	C-O	5.25	1.33	1.23
2	B	59	LYS	C-O	5.20	1.33	1.23
1	A	373	TRP	CB-CG	5.18	1.59	1.50
2	B	155	ALA	C-O	-5.18	1.13	1.23
1	A	220	PHE	CB-CG	5.16	1.60	1.51
2	B	204	GLU	CB-CG	5.15	1.61	1.52
1	A	422	GLU	CD-OE1	5.14	1.31	1.25
2	B	119	GLU	CB-CG	5.14	1.61	1.52
1	A	326	GLU	CD-OE1	5.06	1.31	1.25
1	A	402	LEU	CG-CD2	5.05	1.70	1.51
3	C	77	GLU	C-O	5.04	1.32	1.23
1	A	393	LEU	CG-CD2	5.02	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	96	TYR	CG-CD1	5.00	1.45	1.39

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASN	N-CA-C	8.92	135.08	111.00
1	A	233	ARG	NE-CZ-NH1	8.24	124.42	120.30
3	C	25	ASP	CB-CG-OD2	-8.13	110.99	118.30
2	B	191	ASP	CB-CG-OD1	-8.11	111.00	118.30
2	B	238	LEU	CB-CG-CD2	-7.67	97.97	111.00
2	B	100	LEU	CB-CG-CD1	-7.66	97.98	111.00
2	B	131	LEU	CB-CG-CD2	-7.65	98.00	111.00
3	C	25	ASP	CB-CG-OD1	7.65	125.18	118.30
1	A	453	ARG	NE-CZ-NH1	-7.63	116.49	120.30
3	C	13	ASP	CB-CG-OD1	7.53	125.08	118.30
3	C	12	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	A	133	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	A	339	ARG	C-N-CD	7.05	143.21	128.40
1	A	248	ASN	C-N-CA	-7.03	107.54	122.30
1	A	156	ASP	CB-CG-OD1	-6.92	112.07	118.30
2	B	104	LEU	CB-CG-CD2	-6.72	99.58	111.00
1	A	156	ASP	CB-CG-OD2	6.71	124.34	118.30
2	B	84	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	B	100	LEU	CA-CB-CG	6.50	130.25	115.30
2	B	263	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	A	191	MET	CB-CG-SD	6.48	131.84	112.40
1	A	481	ASP	CB-CG-OD1	6.48	124.13	118.30
2	B	174	ARG	NE-CZ-NH2	6.47	123.53	120.30
1	A	286	ARG	NE-CZ-NH2	-6.43	117.08	120.30
3	C	66	MET	CG-SD-CE	6.38	110.41	100.20
2	B	227	LYS	C-N-CD	6.36	141.76	128.40
1	A	153	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	192	LEU	CB-CG-CD1	-6.22	100.43	111.00
2	B	44	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	286	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	464	LEU	CB-CG-CD2	-6.03	100.75	111.00
2	B	191	ASP	CB-CG-OD2	6.03	123.72	118.30
2	B	76	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	A	450	LEU	CB-CG-CD2	-5.97	100.85	111.00
3	C	28	ASP	CB-CG-OD1	5.95	123.65	118.30
2	B	196	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	233	ARG	NE-CZ-NH2	-5.74	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	ASP	CB-CG-OD1	5.74	123.47	118.30
2	B	104	LEU	CA-CB-CG	-5.71	102.17	115.30
1	A	48	ASP	CB-CG-OD1	5.68	123.41	118.30
2	B	282	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	B	44	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	206	LEU	CB-CG-CD1	5.62	120.56	111.00
2	B	208	LYS	CD-CE-NZ	5.61	124.60	111.70
2	B	162	HIS	N-CA-CB	5.60	120.67	110.60
2	B	225	VAL	CB-CA-C	-5.53	100.89	111.40
2	B	249	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	A	63	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	C	73	LEU	CB-CG-CD2	5.44	120.25	111.00
2	B	37	TYR	CD1-CE1-CZ	-5.43	114.91	119.80
1	A	339	ARG	NE-CZ-NH1	-5.30	117.65	120.30
2	B	32	SER	CB-CA-C	-5.29	100.05	110.10
1	A	453	ARG	NE-CZ-NH2	5.28	122.94	120.30
2	B	300	ILE	CB-CA-C	-5.16	101.28	111.60
1	A	116	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	283	LEU	CA-CB-CG	5.14	127.12	115.30
2	B	300	ILE	CG1-CB-CG2	-5.12	100.14	111.40
1	A	278	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	345	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	230	ASP	CB-CA-C	-5.09	100.23	110.40
1	A	345	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	146	TYR	CB-CG-CD1	-5.05	117.97	121.00
2	B	89	LEU	CA-CB-CG	5.04	126.89	115.30
2	B	322	ARG	N-CA-CB	-5.03	101.54	110.60
1	A	14	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	113	ARG	NE-CZ-NH2	5.03	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	286	ARG	Peptide

## 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	4035	0	3782	163	0
2	B	2641	0	2537	92	0
3	C	676	0	667	50	0
4	A	12	0	15	4	0
5	A	19	0	25	20	0
6	A	2	0	0	0	0
7	B	13	0	15	2	0
8	A	82	0	0	7	0
8	B	72	0	0	2	0
8	C	4	0	0	0	0
All	All	7556	0	7041	273	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 19.

All (273) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:HIS:HE1	2:B:227:LYS:NZ	1.33	1.23
1:A:372:CYS:HB3	3:C:42:ARG:HG2	1.25	1.11
2:B:162:HIS:CE1	2:B:227:LYS:NZ	2.20	1.10
2:B:72:TRP:H	7:B:4401:MPO:H71	1.19	1.05
1:A:427:HIS:HE1	3:C:76:THR:HG23	1.19	1.02
1:A:425:LEU:HD23	3:C:76:THR:HG22	1.42	1.01
1:A:427:HIS:CE1	3:C:76:THR:HG23	1.96	1.00
3:C:28:ASP:OD1	3:C:64:ARG:HB3	1.61	1.00
2:B:162:HIS:CE1	2:B:227:LYS:HZ3	1.76	1.00
1:A:427:HIS:HE1	3:C:76:THR:CG2	1.75	0.99
5:A:4974:P6G:H172	2:B:54:MET:HE1	1.46	0.97
3:C:75:PRO:O	3:C:76:THR:HB	1.64	0.97
2:B:111:GLN:H	2:B:111:GLN:NE2	1.63	0.95
2:B:168:HIS:HD2	2:B:257:GLN:HE21	1.16	0.94
1:A:113:ARG:HH11	2:B:144:GLN:HE21	1.19	0.88
3:C:50:ILE:HD13	3:C:64:ARG:HH12	1.43	0.83
3:C:54:ARG:HG3	3:C:80:ASP:HB2	1.59	0.83
2:B:162:HIS:CE1	2:B:227:LYS:HZ2	1.93	0.83
2:B:162:HIS:HE1	2:B:227:LYS:HZ3	0.85	0.82
3:C:50:ILE:HD13	3:C:64:ARG:NH1	1.94	0.82
2:B:249:LEU:C	2:B:249:LEU:HD23	1.99	0.81
2:B:77:ASP:HB2	2:B:154:CYS:SG	2.20	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:PRO:O	1:A:478:MET:HB3	1.80	0.80
3:C:6:ILE:HG13	3:C:19:VAL:O	1.83	0.79
1:A:387:LEU:HD23	3:C:40:ASN:O	1.83	0.78
2:B:168:HIS:CD2	2:B:257:GLN:HE21	2.02	0.77
5:A:4974:P6G:H172	2:B:54:MET:CE	2.14	0.77
5:A:4974:P6G:C17	2:B:54:MET:HE1	2.14	0.76
3:C:13:ASP:OD1	3:C:42:ARG:HD2	1.85	0.76
5:A:4974:P6G:C17	2:B:54:MET:CE	2.64	0.75
3:C:46:GLN:O	3:C:49:LYS:HB2	1.87	0.73
1:A:314:PRO:HD2	1:A:317:TRP:CE3	2.27	0.70
1:A:139:GLN:HE22	2:B:83:TYR:H	1.39	0.70
5:A:4974:P6G:H151	8:A:4987:HOH:O	1.92	0.69
1:A:127:ALA:CA	1:A:237:GLN:HE22	2.05	0.69
3:C:67:ILE:HG13	3:C:70:ASP:OD2	1.92	0.69
1:A:50:PRO:HD2	1:A:236:GLN:OE1	1.94	0.68
1:A:305:GLN:HE21	1:A:305:GLN:HA	1.59	0.68
1:A:441:PRO:O	1:A:445:LYS:HG3	1.94	0.68
1:A:116:ARG:HD2	1:A:116:ARG:O	1.94	0.68
5:A:4974:P6G:H181	2:B:54:MET:HA	1.76	0.68
1:A:418:GLN:HE22	3:C:78:THR:H	1.41	0.68
1:A:336:TRP:O	1:A:339:ARG:HG2	1.94	0.67
3:C:75:PRO:O	3:C:76:THR:CB	2.41	0.67
2:B:117:TRP:CE3	2:B:245:GLU:HG2	2.30	0.66
3:C:11:GLU:HG2	3:C:12:ARG:HG3	1.75	0.66
1:A:113:ARG:HH11	2:B:144:GLN:NE2	1.90	0.66
1:A:416:ASP:OD2	1:A:427:HIS:HD2	1.77	0.66
2:B:220:THR:HA	2:B:224:LEU:HD12	1.78	0.65
1:A:398:ASN:HD22	1:A:427:HIS:H	1.45	0.64
2:B:145:ILE:HG23	2:B:215:TRP:HB2	1.79	0.64
1:A:491:TYR:O	1:A:492:GLN:HB2	1.97	0.64
2:B:111:GLN:H	2:B:111:GLN:HE21	1.44	0.64
2:B:111:GLN:NE2	2:B:111:GLN:N	2.42	0.64
1:A:372:CYS:HB3	3:C:42:ARG:CG	2.15	0.64
5:A:4974:P6G:H181	2:B:54:MET:CA	2.29	0.63
1:A:427:HIS:CE1	3:C:76:THR:CG2	2.65	0.62
2:B:117:TRP:CZ2	2:B:242:ALA:HA	2.34	0.62
2:B:72:TRP:N	7:B:4401:MPO:H71	2.04	0.62
1:A:116:ARG:NH2	2:B:210:LEU:O	2.33	0.62
1:A:317:TRP:O	1:A:321:MET:HG2	1.99	0.62
3:C:26:THR:HG22	3:C:64:ARG:O	2.01	0.61
1:A:127:ALA:N	1:A:237:GLN:NE2	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:ASP:O	3:C:67:ILE:HG22	2.02	0.60
1:A:368:THR:CG2	1:A:411:LYS:HG2	2.32	0.60
1:A:21:LYS:HE3	1:A:22:TYR:CZ	2.37	0.59
3:C:25:ASP:OD2	3:C:33:LYS:NZ	2.30	0.59
2:B:33:THR:HB	2:B:34:ASN:HD22	1.65	0.59
1:A:2:SER:N	2:B:105:ASN:HD22	2.01	0.59
1:A:127:ALA:HA	1:A:237:GLN:HE22	1.67	0.59
3:C:57:GLU:OE1	3:C:74:ARG:NH2	2.35	0.59
3:C:51:LEU:HA	3:C:82:ILE:O	2.02	0.59
1:A:2:SER:HB2	2:B:105:ASN:HD21	1.67	0.59
1:A:100[B]:TRP:CH2	4:A:4975:GOL:H31	2.38	0.58
2:B:206:ILE:HD13	2:B:226:THR:HG21	1.86	0.58
2:B:311:GLU:O	2:B:315:VAL:HG23	2.03	0.58
2:B:154:CYS:HB3	2:B:267:TRP:CE2	2.39	0.58
1:A:24:THR:OG1	1:A:27:GLU:HG3	2.05	0.57
1:A:318:ASP:O	1:A:321:MET:HB2	2.04	0.56
1:A:357:TRP:CZ2	1:A:361:LYS:HG3	2.40	0.56
1:A:135:ASN:O	1:A:139:GLN:HG3	2.04	0.56
1:A:351:SER:OG	1:A:354:GLU:HG3	2.05	0.56
1:A:2:SER:HB2	2:B:105:ASN:ND2	2.21	0.55
1:A:379:ASN:HD22	1:A:384:LYS:HB2	1.71	0.55
1:A:387:LEU:CD2	3:C:40:ASN:O	2.55	0.55
1:A:191:MET:O	1:A:195:ALA:HB3	2.06	0.55
3:C:50:ILE:HB	3:C:85:ASP:HA	1.88	0.55
1:A:22:TYR:CD1	2:B:204:GLU:HB2	2.42	0.55
1:A:133:ASP:OD2	1:A:233:ARG:HD2	2.07	0.55
1:A:225:SER:O	1:A:229:THR:HG23	2.07	0.55
3:C:26:THR:HA	3:C:66:MET:O	2.07	0.54
5:A:4974:P6G:C17	2:B:54:MET:HE2	2.36	0.54
1:A:304:ARG:HA	1:A:304:ARG:HE	1.72	0.54
1:A:357:TRP:CH2	1:A:361:LYS:HG3	2.41	0.54
3:C:74:ARG:O	3:C:75:PRO:C	2.43	0.54
1:A:416:ASP:OD2	1:A:427:HIS:CD2	2.59	0.54
5:A:4974:P6G:H171	2:B:54:MET:HE2	1.89	0.54
1:A:204:GLN:HB2	1:A:269:PHE:HZ	1.73	0.54
1:A:303:GLU:OE1	1:A:313:LYS:HE2	2.08	0.53
2:B:143:HIS:C	2:B:143:HIS:CD2	2.81	0.53
2:B:180:TYR:N	2:B:181:PRO:HD3	2.24	0.53
3:C:13:ASP:OD2	3:C:42:ARG:NH1	2.41	0.53
1:A:100[B]:TRP:CZ3	4:A:4975:GOL:H31	2.43	0.53
1:A:474:GLU:O	1:A:478:MET:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:MET:O	1:A:299:VAL:HG23	2.08	0.53
3:C:25:ASP:O	3:C:67:ILE:HA	2.09	0.53
1:A:223:LEU:HD23	1:A:224:ILE:HD13	1.90	0.52
1:A:243:LYS:HG3	1:A:309:LEU:CD1	2.40	0.52
2:B:27:GLU:O	2:B:31:VAL:HG22	2.10	0.52
2:B:220:THR:HG21	2:B:288:TRP:HB3	1.92	0.52
2:B:249:LEU:C	2:B:249:LEU:CD2	2.75	0.52
2:B:249:LEU:HD23	2:B:249:LEU:O	2.09	0.52
1:A:96:HIS:O	1:A:100[A]:TRP:CD1	2.63	0.51
1:A:109:THR:HG23	2:B:144:GLN:HB2	1.91	0.51
1:A:139:GLN:NE2	2:B:83:TYR:H	2.06	0.51
2:B:94:GLU:OE1	2:B:168:HIS:HE1	1.94	0.51
1:A:416:ASP:HB2	3:C:16:ILE:CD1	2.40	0.51
1:A:127:ALA:CA	1:A:237:GLN:NE2	2.74	0.51
1:A:86:ASP:OD1	1:A:88:GLY:N	2.43	0.51
1:A:385:PRO:O	1:A:388:THR:N	2.38	0.51
1:A:32:GLU:OE1	5:A:4974:P6G:O19	2.29	0.51
2:B:145:ILE:HG13	2:B:145:ILE:O	2.11	0.51
1:A:345:ASP:HB3	1:A:482:ALA:HA	1.92	0.50
2:B:12:LEU:CD1	2:B:16:SER:HA	2.41	0.50
1:A:184:ASP:H	5:A:4974:P6G:H122	1.76	0.50
2:B:296:ALA:O	2:B:300:ILE:HD12	2.12	0.50
1:A:355:ARG:NH1	1:A:366:ASN:OD1	2.37	0.50
1:A:384:LYS:HB3	1:A:387:LEU:HD13	1.93	0.50
1:A:23:VAL:HG22	2:B:207:GLU:HB3	1.93	0.50
1:A:268:LEU:HG	1:A:272:LEU:HD12	1.94	0.50
1:A:379:ASN:ND2	1:A:384:LYS:HD3	2.27	0.50
1:A:386:GLU:HG2	1:A:387:LEU:HD12	1.93	0.50
2:B:127:PRO:HA	2:B:189:GLU:HB3	1.93	0.49
1:A:103:GLU:CG	1:A:176:PHE:CD2	2.96	0.49
1:A:443:ARG:HG3	2:B:52:LEU:HD11	1.93	0.49
1:A:449:ASN:OD1	1:A:449:ASN:C	2.51	0.49
1:A:296:GLU:HG2	1:A:297:TRP:CD1	2.47	0.49
1:A:206:LEU:HD13	1:A:228:GLN:HG2	1.93	0.49
1:A:167:TRP:HB3	1:A:450:LEU:CD2	2.42	0.49
1:A:359:GLU:OE1	1:A:366:ASN:HB2	2.13	0.49
1:A:273:THR:HA	4:A:3287:GOL:H32	1.95	0.49
1:A:13:THR:O	2:B:166:LEU:HD21	2.13	0.49
1:A:379:ASN:HD22	1:A:384:LYS:HD3	1.77	0.49
3:C:14:PHE:CE2	3:C:42:ARG:HD3	2.48	0.48
1:A:30:PRO:O	1:A:34:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ASP:HB2	8:A:4990:HOH:O	2.13	0.48
3:C:35:ALA:O	3:C:36:TYR:C	2.50	0.48
1:A:34:SER:O	1:A:185:SER:HB3	2.14	0.48
1:A:274:GLY:HA2	1:A:290:PHE:CG	2.49	0.48
2:B:226:THR:O	2:B:227:LYS:C	2.52	0.48
3:C:7:MET:HG2	3:C:76:THR:O	2.13	0.48
3:C:11:GLU:CG	3:C:12:ARG:HG3	2.44	0.48
3:C:63:PRO:HD2	3:C:66:MET:HB3	1.96	0.48
2:B:204:GLU:O	2:B:208:LYS:HB2	2.12	0.48
2:B:154:CYS:HB3	2:B:267:TRP:CD2	2.49	0.48
2:B:66:PRO:HG2	2:B:288:TRP:CZ2	2.49	0.47
2:B:117:TRP:NE1	2:B:247:ASP:HB2	2.29	0.47
1:A:417:TYR:O	1:A:428:PHE:HB2	2.14	0.47
2:B:133:HIS:O	2:B:136:GLN:HB3	2.15	0.47
3:C:54:ARG:CG	3:C:80:ASP:HB2	2.38	0.47
1:A:127:ALA:HB2	1:A:237:GLN:NE2	2.30	0.46
1:A:153:ARG:NH2	8:A:4995:HOH:O	2.45	0.46
1:A:244:ILE:O	1:A:244:ILE:HG13	2.08	0.46
1:A:204:GLN:HB2	1:A:269:PHE:CZ	2.51	0.46
1:A:461:PRO:O	1:A:466:GLY:HA3	2.15	0.46
2:B:21:ASN:C	2:B:23:ARG:H	2.18	0.46
1:A:89:TRP:O	1:A:90:VAL:C	2.51	0.46
1:A:103:GLU:HG3	1:A:176:PHE:CD2	2.51	0.46
1:A:339:ARG:NH1	1:A:485:TYR:OH	2.48	0.46
1:A:33:MET:SD	5:A:4974:P6G:H182	2.56	0.46
2:B:128:ALA:HB2	8:B:4436:HOH:O	2.15	0.46
1:A:368:THR:HB	1:A:408:PRO:HD2	1.98	0.46
1:A:317:TRP:O	1:A:320:PHE:HB3	2.15	0.46
1:A:300:ALA:HB3	1:A:301:GLN:OE1	2.15	0.45
1:A:443:ARG:HA	2:B:52:LEU:HD21	1.99	0.45
1:A:467:ALA:O	1:A:468:LEU:C	2.54	0.45
3:C:50:ILE:N	3:C:84:MET:O	2.25	0.45
1:A:339:ARG:HD2	1:A:480:ASP:HA	1.98	0.45
2:B:131:LEU:O	2:B:134:ALA:HB3	2.17	0.45
1:A:395:THR:OG1	3:C:16:ILE:HG22	2.17	0.45
1:A:96:HIS:O	1:A:100[B]:TRP:HB2	2.17	0.45
2:B:245:GLU:HG3	8:B:4454:HOH:O	2.16	0.45
1:A:47:TYR:CE1	1:A:240:PRO:HB2	2.52	0.45
1:A:183:ARG:HH11	5:A:4974:P6G:C9	2.30	0.45
2:B:179:CYS:C	2:B:181:PRO:HD3	2.37	0.45
1:A:449:ASN:OD1	1:A:451:VAL:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:NH1	5:A:4974:P6G:H91	2.33	0.44
1:A:204:GLN:NE2	4:A:3287:GOL:H11	2.32	0.44
1:A:275:PRO:HD3	1:A:328:HIS:HB2	1.99	0.44
1:A:338:TRP:CD1	1:A:390:PRO:HG3	2.53	0.44
1:A:153:ARG:NH1	2:B:12:LEU:HD21	2.32	0.44
2:B:43:GLU:CD	2:B:43:GLU:H	2.21	0.44
1:A:21:LYS:HG2	1:A:22:TYR:CE2	2.52	0.44
1:A:39:ILE:HD13	1:A:248:ASN:HB2	1.99	0.44
1:A:113:ARG:NH1	2:B:144:GLN:HE21	2.01	0.44
1:A:39:ILE:HB	1:A:44:TRP:HE1	1.83	0.44
3:C:19:VAL:HG12	3:C:20:PRO:O	2.18	0.44
3:C:27:MET:HG3	3:C:62:PHE:HB2	1.98	0.44
1:A:231:GLU:HG3	1:A:235:ALA:HB2	2.00	0.44
1:A:258:VAL:O	1:A:262:ILE:HG13	2.17	0.44
2:B:57:TRP:HZ2	2:B:141:TYR:HH	1.62	0.44
2:B:109:HIS:HD2	2:B:248:THR:HG23	1.83	0.44
1:A:183:ARG:O	8:A:4994:HOH:O	2.21	0.44
1:A:197:GLU:CD	1:A:231:GLU:OE2	2.55	0.44
1:A:203:MET:O	1:A:204:GLN:C	2.56	0.44
2:B:104:LEU:HD23	2:B:104:LEU:HA	1.32	0.43
1:A:39:ILE:HB	1:A:44:TRP:NE1	2.34	0.43
1:A:134:GLU:OE2	1:A:134:GLU:HA	2.17	0.43
1:A:421:TYR:HE2	1:A:445:LYS:HE2	1.83	0.43
2:B:263:ARG:HB2	2:B:266:ARG:NH2	2.34	0.43
3:C:55:ARG:HD2	3:C:58:ASP:OD1	2.18	0.43
1:A:223:LEU:CD2	1:A:224:ILE:HD13	2.47	0.43
2:B:241:LEU:O	2:B:245:GLU:HB2	2.19	0.43
1:A:416:ASP:HB2	3:C:16:ILE:HD12	2.01	0.43
2:B:168:HIS:HD2	2:B:257:GLN:NE2	1.99	0.43
1:A:314:PRO:HB3	1:A:316:TYR:CE2	2.53	0.43
1:A:334:GLY:O	1:A:338:TRP:HB2	2.19	0.43
5:A:4974:P6G:H81	5:A:4974:P6G:H111	1.42	0.43
1:A:152:SER:HB3	1:A:155:TRP:CD1	2.53	0.43
1:A:165:ASN:HB3	1:A:170:ILE:HD11	2.01	0.43
1:A:22:TYR:CG	2:B:204:GLU:HB2	2.54	0.42
1:A:116:ARG:HG2	2:B:141:TYR:HB2	2.00	0.42
5:A:4974:P6G:H52	5:A:4974:P6G:H82	1.53	0.42
5:A:4974:P6G:C18	2:B:54:MET:HE1	2.49	0.42
8:A:5005:HOH:O	2:B:36:HIS:HD2	2.02	0.42
1:A:121:PRO:HD2	8:A:4986:HOH:O	2.19	0.42
2:B:137:MET:HE2	2:B:210:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:CD2	1:A:22:TYR:N	2.87	0.42
2:B:131:LEU:O	2:B:131:LEU:HD12	2.20	0.42
3:C:30:VAL:HG12	3:C:31:ALA:N	2.34	0.42
3:C:52:ARG:NH2	3:C:61:LEU:HG	2.35	0.42
1:A:103:GLU:CD	1:A:176:PHE:CD2	2.93	0.42
1:A:299:VAL:O	1:A:303:GLU:CG	2.68	0.42
1:A:123:ASN:ND2	8:A:5006:HOH:O	2.52	0.42
1:A:418:GLN:NE2	3:C:78:THR:H	2.12	0.42
2:B:250:LEU:HD12	2:B:250:LEU:O	2.20	0.42
1:A:212:ALA:HB2	1:A:220:PHE:HD2	1.85	0.42
1:A:416:ASP:OD1	1:A:416:ASP:C	2.58	0.42
5:A:4974:P6G:H171	2:B:54:MET:HB2	2.02	0.42
2:B:305:SER:HB3	2:B:314:ILE:HD11	2.02	0.42
3:C:44:HIS:HA	3:C:45:PRO:HD2	1.76	0.42
1:A:183:ARG:HH11	5:A:4974:P6G:H91	1.85	0.42
1:A:411:LYS:HB3	1:A:411:LYS:NZ	2.35	0.42
5:A:4974:P6G:C18	2:B:54:MET:CE	2.98	0.42
1:A:178:ASP:O	1:A:183:ARG:HG2	2.20	0.41
2:B:190:ARG:O	2:B:194:GLU:N	2.36	0.41
1:A:6:ARG:C	1:A:8:ASP:N	2.74	0.41
2:B:145:ILE:HG23	2:B:215:TRP:CB	2.47	0.41
1:A:249:GLY:C	1:A:250:LYS:HG2	2.41	0.41
1:A:402:LEU:HB3	1:A:403:PRO:HD2	2.02	0.41
1:A:260:VAL:O	1:A:264:ARG:HG3	2.20	0.41
1:A:449:ASN:O	1:A:452:ASP:HB2	2.20	0.41
2:B:223:ASN:O	2:B:228:PRO:HD3	2.20	0.41
1:A:191:MET:SD	1:A:257:MET:HB3	2.61	0.41
2:B:293:GLU:O	2:B:294:PRO:C	2.58	0.41
3:C:6:ILE:HD11	3:C:19:VAL:HB	2.01	0.41
1:A:396:ILE:HG22	1:A:397:CYS:O	2.21	0.41
1:A:478:MET:HG3	1:A:478:MET:H	1.72	0.41
3:C:23:THR:HA	3:C:68:VAL:CG1	2.50	0.41
1:A:2:SER:N	2:B:102:ASP:O	2.54	0.41
1:A:47:TYR:CD2	1:A:47:TYR:C	2.94	0.41
1:A:12:LEU:HD11	2:B:174:ARG:NH1	2.36	0.41
1:A:19:THR:HA	1:A:20:PRO:HD2	1.83	0.41
1:A:297:TRP:HA	1:A:301:GLN:HE22	1.86	0.41
1:A:68:GLY:O	1:A:71:SER:HB2	2.21	0.41
1:A:153:ARG:CZ	2:B:12:LEU:HD21	2.52	0.40
1:A:364:GLY:O	1:A:365:TRP:C	2.57	0.40
1:A:400:CYS:O	1:A:401:ASN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:LEU:HB3	1:A:403:PRO:CD	2.51	0.40
1:A:325:ASP:O	1:A:329:HIS:HD2	2.04	0.40
1:A:201:THR:O	1:A:205:PHE:HB2	2.22	0.40
1:A:398:ASN:ND2	1:A:427:HIS:H	2.16	0.40
1:A:127:ALA:CB	1:A:237:GLN:HE22	2.34	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	490/498 (98%)	442 (90%)	44 (9%)	4 (1%)	19	15
2	B	320/330 (97%)	292 (91%)	25 (8%)	3 (1%)	17	12
3	C	81/86 (94%)	70 (86%)	9 (11%)	2 (2%)	5	2
All	All	891/914 (98%)	804 (90%)	78 (9%)	9 (1%)	15	11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	GLU
1	A	287	ASN
2	B	310	GLY
1	A	408	PRO
1	A	445	LYS
2	B	327	MET
3	C	77	GLU
2	B	22	ARG
3	C	31	ALA

### 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	418/422 (99%)	393 (94%)	25 (6%)	19	16
2	B	274/282 (97%)	252 (92%)	22 (8%)	12	8
3	C	77/79 (98%)	66 (86%)	11 (14%)	3	1
All	All	769/783 (98%)	711 (92%)	58 (8%)	13	10

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	34	SER
1	A	77	GLU
1	A	78	ARG
1	A	153	ARG
1	A	206	LEU
1	A	223	LEU
1	A	226	SER
1	A	228	GLN
1	A	233	ARG
1	A	243	LYS
1	A	244	ILE
1	A	256	GLN
1	A	280	TYR
1	A	283	LEU
1	A	287	ASN
1	A	303	GLU
1	A	305	GLN
1	A	309	LEU
1	A	407	THR
1	A	411	LYS
1	A	419	LEU
1	A	464	LEU
1	A	477	VAL
1	A	478	MET
2	B	13	LYS

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Mol	Chain	Res	Type
2	B	22	ARG
2	B	23	ARG
2	B	43	GLU
2	B	89	LEU
2	B	100	LEU
2	B	109	HIS
2	B	111	GLN
2	B	113	LEU
2	B	116	GLU
2	B	140	VAL
2	B	143	HIS
2	B	188	ARG
2	B	200	GLN
2	B	240	SER
2	B	248	THR
2	B	278	LYS
2	B	279	GLU
2	B	284	VAL
2	B	293	GLU
2	B	298	LYS
2	B	309	ASP
3	C	3	THR
3	C	5	PRO
3	C	12	ARG
3	C	25	ASP
3	C	26	THR
3	C	66	MET
3	C	67	ILE
3	C	70	ASP
3	C	76	THR
3	C	84	MET
3	C	85	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	139	GLN
1	A	237	GLN
1	A	248	ASN
1	A	305	GLN
1	A	379	ASN

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Mol	Chain	Res	Type
1	A	398	ASN
1	A	418	GLN
1	A	427	HIS
2	B	34	ASN
2	B	36	HIS
2	B	87	ASN
2	B	105	ASN
2	B	111	GLN
2	B	144	GLN
2	B	153	ASN
2	B	162	HIS
2	B	168	HIS
3	C	56	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
7	MPO	B	4401	-	13,13,13	3.05	7 (53%)	17,17,17	4.23	10 (58%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	P6G	A	4974	-	18,18,18	1.47	3 (16%)	17,17,17	1.29	3 (17%)
4	GOL	A	4975	6	5,5,5	1.03	0	5,5,5	1.75	2 (40%)
4	GOL	A	3287	-	5,5,5	0.39	0	5,5,5	0.93	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
7	MPO	B	4401	-	-	5/7/15/15	0/1/1/1
5	P6G	A	4974	-	-	12/16/16/16	-
4	GOL	A	4975	6	-	2/4/4/4	-
4	GOL	A	3287	-	-	3/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4401	MPO	C4-N1	-5.35	1.32	1.46
7	B	4401	MPO	O2-S1	5.26	1.60	1.45
7	B	4401	MPO	C4-C5	-4.01	1.34	1.50
7	B	4401	MPO	O1-S1	3.93	1.56	1.45
5	A	4974	P6G	O19-C18	-3.74	1.22	1.42
7	B	4401	MPO	C3-N1	3.06	1.54	1.47
7	B	4401	MPO	C1-S1	-2.85	1.73	1.77
5	A	4974	P6G	C15-C14	2.30	1.60	1.49
5	A	4974	P6G	O13-C14	2.19	1.51	1.42
7	B	4401	MPO	C2-C3	2.16	1.60	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4401	MPO	O2-S1-C1	9.50	118.35	106.92
7	B	4401	MPO	C5-C4-N1	7.54	121.54	110.10
7	B	4401	MPO	O3-S1-O2	-6.35	95.76	111.27
7	B	4401	MPO	C7-N1-C4	4.45	118.85	108.83
7	B	4401	MPO	C3-N1-C4	4.27	122.14	111.23
7	B	4401	MPO	C3-C2-C1	4.22	127.90	113.14
7	B	4401	MPO	C6-O4-C5	4.12	123.63	109.89
7	B	4401	MPO	C2-C1-S1	4.03	119.42	113.25
7	B	4401	MPO	C3-N1-C7	3.04	119.00	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	4401	MPO	O4-C6-C7	-2.74	105.77	111.80
4	A	4975	GOL	O2-C2-C3	2.71	121.06	109.12
5	A	4974	P6G	O16-C15-C14	2.57	121.96	110.39
5	A	4974	P6G	O16-C17-C18	2.42	120.71	110.07
5	A	4974	P6G	O19-C18-C17	2.28	125.06	111.81
4	A	4975	GOL	O2-C2-C1	2.25	119.04	109.12

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4975	GOL	C1-C2-C3-O3
4	A	3287	GOL	O1-C1-C2-C3
5	A	4974	P6G	C8-C9-O10-C11
7	B	4401	MPO	C2-C3-N1-C4
5	A	4974	P6G	C5-C6-O7-C8
5	A	4974	P6G	O13-C14-C15-O16
5	A	4974	P6G	O7-C8-C9-O10
5	A	4974	P6G	O1-C2-C3-O4
5	A	4974	P6G	O16-C17-C18-O19
5	A	4974	P6G	C15-C14-O13-C12
4	A	4975	GOL	O2-C2-C3-O3
4	A	3287	GOL	O1-C1-C2-O2
5	A	4974	P6G	O10-C11-C12-O13
7	B	4401	MPO	C2-C1-S1-O1
7	B	4401	MPO	C2-C1-S1-O2
7	B	4401	MPO	C2-C1-S1-O3
5	A	4974	P6G	O4-C5-C6-O7
5	A	4974	P6G	C11-C12-O13-C14
5	A	4974	P6G	C2-C3-O4-C5
7	B	4401	MPO	C1-C2-C3-N1
4	A	3287	GOL	O2-C2-C3-O3
5	A	4974	P6G	C12-C11-O10-C9

There are no ring outliers.

4 monomers are involved in 26 short contacts:

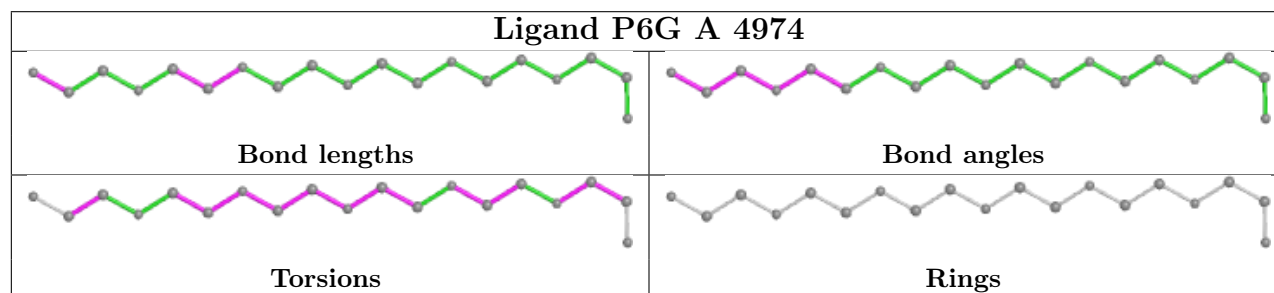
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	4401	MPO	2	0
5	A	4974	P6G	20	0
4	A	4975	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3287	GOL	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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	491/498 (98%)	0.07	25 (5%) 28 33	33, 50, 65, 81	0
2	B	322/330 (97%)	-0.09	17 (5%) 26 32	33, 45, 65, 92	0
3	C	83/86 (96%)	0.05	3 (3%) 42 49	48, 63, 78, 85	0
All	All	896/914 (98%)	0.01	45 (5%) 28 34	33, 49, 69, 92	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100[A]	TRP	6.1
2	B	8	ALA	5.7
2	B	23	ARG	5.0
2	B	22	ARG	4.9
1	A	268	LEU	4.3
1	A	176	PHE	3.7
2	B	21	ASN	3.6
1	A	107	ALA	3.4
2	B	140	VAL	3.3
1	A	272	LEU	3.3
1	A	490	ALA	3.2
2	B	311	GLU	3.2
1	A	381	VAL	3.2
1	A	108	SER	2.9
3	C	48	GLU	2.8
1	A	109	THR	2.8
2	B	159	THR	2.7
2	B	9	LEU	2.7
2	B	309	ASP	2.7
2	B	10	LYS	2.6
1	A	492	GLN	2.5
3	C	73	LEU	2.5
1	A	423	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	142	ILE	2.5
1	A	128	THR	2.4
2	B	163	LEU	2.4
2	B	160	ALA	2.4
2	B	156	THR	2.4
1	A	175	PHE	2.4
1	A	112	ALA	2.4
1	A	115	ALA	2.4
1	A	304	ARG	2.4
1	A	269	PHE	2.3
1	A	172	ALA	2.3
2	B	152	THR	2.3
1	A	131	MET	2.3
1	A	271	VAL	2.3
2	B	20	GLY	2.2
1	A	265	SER	2.2
1	A	80	GLY	2.2
3	C	85	ASP	2.1
1	A	106	ALA	2.1
1	A	127	ALA	2.1
2	B	139	SER	2.0
1	A	110	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

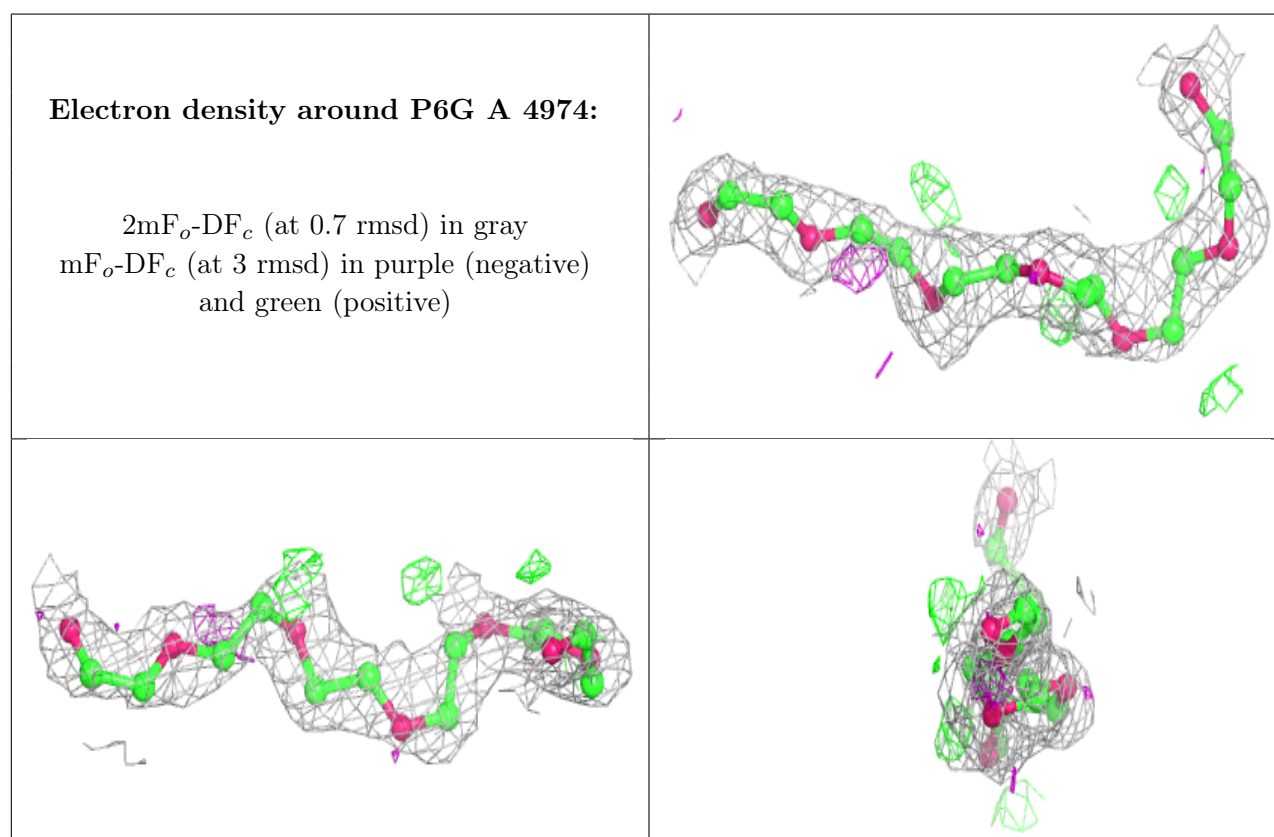
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MPO	B	4401	13/13	0.86	0.17	60,66,72,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	3287	6/6	0.87	0.41	83,87,88,89	0
5	P6G	A	4974	19/19	0.88	0.19	47,56,72,76	0
4	GOL	A	4975	6/6	0.97	0.27	43,57,61,65	0
6	FE	A	500	1/1	0.99	0.13	45,45,45,45	0
6	FE	A	499	1/1	0.99	0.12	39,39,39,39	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.



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

There are no such residues in this entry.