



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:46 am BST

PDB ID : 1RT4  
Title : HIV-1 REVERSE TRANSCRIPTASE COMPLEXED WITH UC781  
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Deposited on : 1998-07-29  
Resolution : 2.90 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 : 2.11  
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) : 2.11

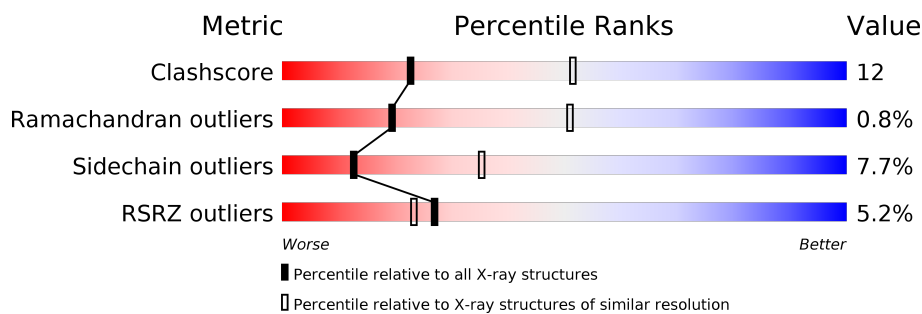
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	560	<div> <div>7%</div> <div>65%</div> <div>27%</div> <div>• •</div> </div>
2	B	440	<div> <div>2%</div> <div>65%</div> <div>24%</div> <div>• 8%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7766 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 HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4396	2847	732	809	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	MODIFIED RESIDUE	UNP P04585

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

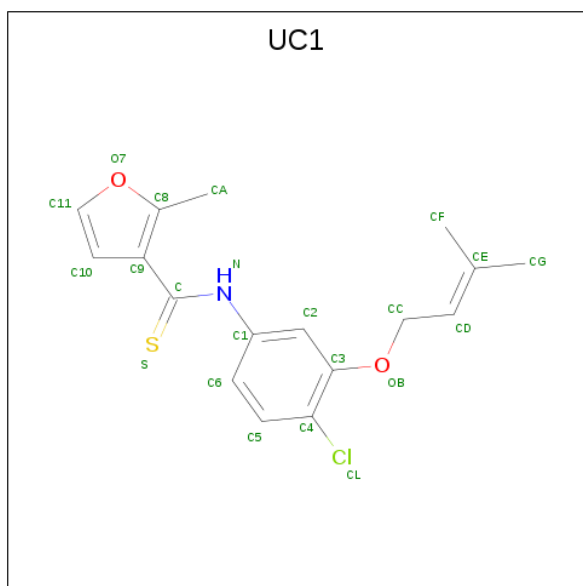
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	404	Total	C	N	O	S	0	0	0
			3340	2170	556	607	7			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 4 is 2-METHYL-FURAN-3-CARBOTHIOIC ACID [4-CHLORO-3-(3-METHYL-BUT-2-ENYLOXY)-PHENYL]-AMIDE (three-letter code: UC1) (formula: C<sub>17</sub>H<sub>18</sub>ClNO<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			22	17	1	1	2	1		

- Molecule 5 is water.

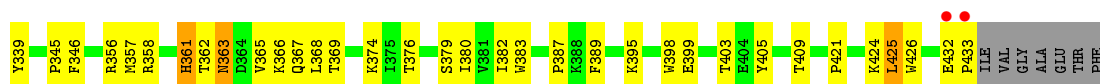
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	1	Total O 1 1	0	0

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

The figure displays a sequence logo for Chain A, illustrating the conservation of amino acids at each position (1 to 70). The y-axis lists the amino acids, categorized by color: Grey (W, K, C, S, G, I, L, N, V), Green (D, E, Q, R, H, Y, F, P, M, T, A, G), Yellow (K, R, D, E, Q, R, H, Y, F, P, M, T, A, G), Orange (Q, R, H, Y, F, P, M, T, A, G), Red (R, H, Y, F, P, M, T, A, G), and Blue (P, M, T, A, G). The x-axis represents the protein positions from 1 to 70. Above the chart, a horizontal bar indicates the overall conservation percentage for each position, ranging from 7% (red) to 27% (yellow). Red dots above specific positions indicate high conservation.

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.40 Å   111.20 Å   73.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.90) 93.6 (29.93-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 2.90 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.237 ,   0.295 0.209 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 87.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: CSD, PO4, UC1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.33	0/4503	0.59	0/6117
2	B	0.32	0/3432	0.61	1/4659 (0.0%)
All	All	0.33	0/7935	0.60	1/10776 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	236	PRO	N-CA-C	5.07	125.27	112.10

There are no chirality outliers.

There are no planarity outliers.

### 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	4396	0	4451	105	0
2	B	3340	0	3376	73	0
3	A	5	0	0	0	0
4	A	22	0	18	7	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
All	All	7766	0	7845	180	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 12.

All (180) 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:278:GLN:HG2	1:A:298:GLU:HB3	1.54	0.89
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.61	0.82
1:A:410:TRP:CD1	2:B:363:ASN:HB2	2.16	0.80
1:A:21:VAL:HG11	1:A:59:PRO:HD3	1.68	0.75
2:B:158:ALA:O	2:B:161:GLN:HB2	1.90	0.72
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.21	0.71
2:B:101:LYS:HE2	2:B:382:ILE:HG23	1.74	0.69
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.75	0.69
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.74	0.68
1:A:109:LEU:HD23	1:A:216:THR:HG21	1.76	0.67
1:A:26:LEU:HD22	1:A:30:LYS:HE2	1.75	0.67
1:A:92:LEU:H	1:A:92:LEU:HD23	1.60	0.66
2:B:101:LYS:HG2	2:B:382:ILE:HA	1.76	0.66
2:B:157:PRO:HG2	2:B:184:MET:HA	1.78	0.66
2:B:395:LYS:O	2:B:399:GLU:HG2	1.95	0.66
1:A:358:ARG:HB3	1:A:358:ARG:NH1	2.11	0.65
1:A:474:ASN:ND2	1:A:474:ASN:H	1.95	0.64
1:A:235:HIS:HB2	1:A:238:LYS:O	1.97	0.64
2:B:242:GLN:HE21	2:B:242:GLN:HA	1.63	0.63
1:A:461:ARG:HH11	1:A:461:ARG:HG3	1.63	0.63
1:A:356:ARG:HH22	1:A:371:ALA:HB2	1.63	0.63
1:A:23:GLN:HE22	1:A:60:VAL:H	1.46	0.62
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.65	0.62
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.35	0.61
2:B:13:LYS:HE2	2:B:82:LYS:O	2.01	0.61
1:A:340:GLN:CB	1:A:351:THR:HG22	2.31	0.60
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.84	0.59
2:B:295:LEU:H	2:B:295:LEU:HD12	1.66	0.59
1:A:171:PHE:HB2	1:A:208:HIS:HD2	1.66	0.59
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.02	0.58
1:A:34:LEU:HB3	1:A:132:ILE:HD12	1.85	0.58
1:A:27:THR:HB	1:A:30:LYS:HG3	1.86	0.58
2:B:363:ASN:ND2	2:B:366:LYS:HB2	2.19	0.58
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.86	0.58
2:B:421:PRO:O	2:B:425:LEU:HD22	2.04	0.57
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.87	0.57
1:A:122:GLU:CD	1:A:122:GLU:H	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:LYS:HA	2:B:374:LYS:HE2	1.86	0.56
1:A:381:VAL:HG22	2:B:25:PRO:HB3	1.88	0.56
2:B:72:ARG:HH21	2:B:409:THR:HG22	1.71	0.56
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.39	0.56
2:B:197:GLN:O	2:B:201:LYS:HB2	2.06	0.56
1:A:64:LYS:HD2	1:A:68:SER:HA	1.89	0.55
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.41	0.55
1:A:489:SER:HB2	1:A:493:VAL:HG22	1.88	0.55
2:B:206:ARG:O	2:B:210:LEU:HD13	2.06	0.55
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.89	0.54
1:A:240:THR:OG1	1:A:315:HIS:HB3	2.08	0.54
2:B:163:SER:O	2:B:167:ILE:HG13	2.08	0.54
2:B:131:THR:OG1	2:B:143:ARG:HD2	2.07	0.53
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.43	0.53
1:A:503:LEU:HA	1:A:506:ILE:HD12	1.89	0.53
1:A:126:LYS:HE3	1:A:127:TYR:CZ	2.44	0.53
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.90	0.53
2:B:356:ARG:NH2	2:B:361:HIS:HB3	2.24	0.53
1:A:21:VAL:HG22	1:A:22:LYS:HD3	1.91	0.52
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.91	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.09	0.52
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.92	0.51
4:A:999:UC1:H2	4:A:999:UC1:HD	1.92	0.51
4:A:999:UC1:H2	4:A:999:UC1:C9	2.41	0.51
2:B:365:VAL:O	2:B:369:THR:HG23	2.11	0.51
1:A:37:ILE:O	1:A:40:GLU:HB3	2.11	0.50
1:A:142:ILE:N	1:A:142:ILE:HD12	2.26	0.50
1:A:358:ARG:HH11	1:A:358:ARG:HB3	1.76	0.50
1:A:542:ILE:HD12	1:A:542:ILE:H	1.77	0.50
1:A:344:GLU:HB2	1:A:347:LYS:HD3	1.94	0.50
1:A:454:LYS:HA	1:A:467:VAL:O	2.11	0.50
1:A:489:SER:HB2	1:A:493:VAL:CG2	2.41	0.49
1:A:94:ILE:HG23	1:A:229:TRP:HZ2	1.76	0.49
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.77	0.49
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.93	0.49
2:B:95:PRO:O	2:B:181:TYR:HE1	1.95	0.49
1:A:362:THR:HG22	1:A:363:ASN:H	1.76	0.49
4:A:999:UC1:H2	4:A:999:UC1:CD	2.43	0.49
2:B:103:LYS:O	2:B:236:PRO:HD2	2.12	0.49
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.11	0.49
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HG13	1:A:283:LEU:HD12	1.95	0.49
1:A:17:ASP:O	1:A:83:ARG:HD3	2.13	0.49
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.13	0.48
1:A:432:GLU:HB2	1:A:433:PRO:HD2	1.96	0.48
1:A:13:LYS:HE3	1:A:84:THR:O	2.13	0.48
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.94	0.48
2:B:361:HIS:HD2	2:B:362:THR:HG23	1.78	0.48
4:A:999:UC1:C10	4:A:999:UC1:C2	2.92	0.48
2:B:5:ILE:HG22	2:B:6:GLU:H	1.78	0.48
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.43	0.47
4:A:999:UC1:H2	4:A:999:UC1:C10	2.44	0.47
1:A:57:ASN:HA	1:A:129:ALA:O	2.15	0.47
1:A:72:ARG:HH21	1:A:74:LEU:HD11	1.79	0.47
1:A:19:PRO:HG2	1:A:80:LEU:HB2	1.96	0.47
2:B:120:LEU:HD12	2:B:150:PRO:HD3	1.97	0.47
1:A:497:THR:O	1:A:535:TRP:HA	2.14	0.47
2:B:379:SER:CB	2:B:387:PRO:HD3	2.44	0.46
2:B:98:ALA:O	2:B:101:LYS:HD3	2.15	0.46
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.50	0.46
1:A:283:LEU:O	1:A:286:THR:HG23	2.16	0.46
1:A:7:THR:HG22	1:A:119:PRO:O	2.16	0.46
2:B:175:ASN:N	2:B:176:PRO:HD3	2.31	0.46
2:B:81:ASN:OD1	2:B:153:TRP:HD1	1.99	0.45
2:B:31:ILE:O	2:B:35:VAL:HG23	2.17	0.45
2:B:356:ARG:HB2	2:B:367:GLN:HG2	1.98	0.45
1:A:234:LEU:HB3	4:A:999:UC1:CL	2.54	0.45
2:B:206:ARG:HH22	2:B:210:LEU:HD21	1.81	0.45
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.81	0.45
1:A:197:GLN:NE2	1:A:197:GLN:HA	2.31	0.45
2:B:66:LYS:HG3	2:B:67:ASP:OD1	2.17	0.45
1:A:13:LYS:HG2	1:A:83:ARG:O	2.17	0.45
1:A:40:GLU:O	1:A:43:LYS:HG2	2.17	0.44
2:B:66:LYS:O	2:B:67:ASP:HB2	2.16	0.44
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.33	0.44
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.83	0.44
1:A:419:THR:O	1:A:419:THR:HG23	2.17	0.44
2:B:244:ILE:HG21	2:B:426:TRP:CH2	2.52	0.44
1:A:111:VAL:HG22	1:A:185:ASP:O	2.17	0.44
1:A:542:ILE:HG12	2:B:283:LEU:HD23	1.99	0.44
2:B:366:LYS:HG2	2:B:405:TYR:CD1	2.52	0.44
2:B:65:LYS:O	2:B:68:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:O	1:A:148:VAL:HG21	2.17	0.44
1:A:218:ASP:O	1:A:222:GLN:HG3	2.17	0.44
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.99	0.44
2:B:63:ILE:HD13	2:B:72:ARG:O	2.17	0.44
1:A:122:GLU:HA	1:A:125:ARG:NE	2.33	0.44
1:A:228:LEU:HD11	1:A:242:GLN:HE22	1.84	0.43
1:A:260:LEU:O	1:A:264:LEU:HD23	2.18	0.43
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.48	0.43
1:A:356:ARG:HB2	1:A:367:GLN:NE2	2.34	0.43
1:A:393:ILE:HB	1:A:423:VAL:HG22	2.01	0.43
1:A:69:THR:HG22	1:A:70:LYS:N	2.33	0.43
4:A:999:UC1:S	4:A:999:UC1:HA1	2.58	0.43
2:B:64:LYS:HD2	2:B:71:TRP:CE2	2.54	0.43
1:A:356:ARG:HE	1:A:374:LYS:HZ3	1.65	0.43
2:B:157:PRO:CG	2:B:184:MET:HA	2.47	0.43
1:A:442:VAL:HG11	1:A:485:ALA:HB2	2.00	0.43
2:B:30:LYS:HE2	2:B:30:LYS:HB3	1.80	0.43
1:A:257:ILE:O	1:A:261:VAL:HG23	2.18	0.42
2:B:171:PHE:O	2:B:175:ASN:HB2	2.19	0.42
1:A:26:LEU:HB3	1:A:30:LYS:HB2	2.00	0.42
1:A:273:GLY:O	1:A:275:LYS:HG3	2.19	0.42
2:B:105:SER:HA	2:B:234:LEU:O	2.18	0.42
2:B:65:LYS:HZ1	2:B:72:ARG:HE	1.66	0.42
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.67	0.42
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.55	0.42
1:A:287:LYS:HG2	1:A:291:GLU:OE2	2.19	0.42
1:A:293:ILE:HD12	1:A:293:ILE:N	2.35	0.42
1:A:11:LYS:HE2	1:A:11:LYS:HB2	1.92	0.42
1:A:439:THR:HG21	2:B:289:LEU:HD13	2.01	0.42
2:B:206:ARG:NH2	2:B:210:LEU:HD21	2.33	0.42
1:A:452:LEU:HD22	1:A:470:THR:HA	2.01	0.42
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.55	0.42
1:A:438:GLU:HG3	1:A:461:ARG:HD2	2.02	0.42
2:B:363:ASN:HD21	2:B:366:LYS:HB2	1.84	0.42
2:B:432:GLU:HB3	2:B:433:PRO:HD2	2.01	0.42
1:A:366:LYS:O	1:A:369:THR:HB	2.20	0.41
2:B:328:GLU:O	2:B:339:TYR:HA	2.20	0.41
1:A:248:GLU:HA	1:A:307:ARG:NH2	2.36	0.41
1:A:475:GLN:HB2	1:A:475:GLN:HE21	1.72	0.41
2:B:93:GLY:O	2:B:94:ILE:HG13	2.20	0.41
1:A:135:ILE:HD13	1:A:135:ILE:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.02	0.41
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.55	0.41
1:A:439:THR:O	1:A:459:THR:HA	2.21	0.41
1:A:73:LYS:O	1:A:74:LEU:HD12	2.19	0.41
2:B:10:VAL:HG11	2:B:153:TRP:CH2	2.56	0.41
1:A:115:TYR:O	1:A:149:LEU:HB2	2.20	0.41
1:A:254:VAL:HG22	1:A:293:ILE:HD11	2.02	0.41
1:A:201:LYS:HD3	1:A:201:LYS:HA	1.91	0.41
1:A:2:ILE:HG22	1:A:3:SER:N	2.36	0.41
2:B:345:PRO:O	2:B:346:PHE:HB2	2.21	0.41
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.56	0.41
2:B:206:ARG:HB3	2:B:206:ARG:NH1	2.35	0.41
2:B:376:THR:O	2:B:380:ILE:HG13	2.21	0.41
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.56	0.40
1:A:356:ARG:HE	1:A:374:LYS:NZ	2.18	0.40
1:A:438:GLU:CG	1:A:461:ARG:HD2	2.51	0.40
1:A:56:TYR:O	1:A:143:ARG:NH2	2.54	0.40
2:B:115:TYR:HB3	2:B:149:LEU:HB2	2.04	0.40
2:B:288:ALA:O	2:B:291:GLU:HB3	2.21	0.40
2:B:78:ARG:O	2:B:82:LYS:HG3	2.21	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	532/560 (95%)	499 (94%)	27 (5%)	6 (1%)	14	42
2	B	398/440 (90%)	378 (95%)	19 (5%)	1 (0%)	41	71
All	All	930/1000 (93%)	877 (94%)	46 (5%)	7 (1%)	19	51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLY
1	A	66	LYS
1	A	92	LEU
1	A	67	ASP
1	A	358	ARG
2	B	361	HIS
1	A	111	VAL

### 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	481/499 (96%)	441 (92%)	40 (8%)	11	32
2	B	368/400 (92%)	343 (93%)	25 (7%)	16	42
All	All	849/899 (94%)	784 (92%)	65 (8%)	13	35

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	53	GLU
1	A	67	ASP
1	A	68	SER
1	A	135	ILE
1	A	197	GLN
1	A	205	LEU
1	A	208	HIS
1	A	211	ARG
1	A	228	LEU
1	A	230	MET
1	A	248	GLU
1	A	251	SER
1	A	263	LYS
1	A	277	ARG
1	A	295	LEU
1	A	296	THR

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Mol	Chain	Res	Type
1	A	297	GLU
1	A	301	LEU
1	A	303	LEU
1	A	311	LYS
1	A	315	HIS
1	A	340	GLN
1	A	347	LYS
1	A	358	ARG
1	A	361	HIS
1	A	362	THR
1	A	368	LEU
1	A	404	GLU
1	A	424	LYS
1	A	431	LYS
1	A	452	LEU
1	A	464	GLN
1	A	474	ASN
1	A	475	GLN
1	A	491	LEU
1	A	496	VAL
1	A	517	LEU
1	A	540	LYS
1	A	542	ILE
2	B	6	GLU
2	B	8	VAL
2	B	24	TRP
2	B	63	ILE
2	B	65	LYS
2	B	69	THR
2	B	72	ARG
2	B	87	PHE
2	B	95	PRO
2	B	101	LYS
2	B	109	LEU
2	B	123	ASP
2	B	139	THR
2	B	186	ASP
2	B	194	GLU
2	B	242	GLN
2	B	263	LYS
2	B	283	LEU
2	B	289	LEU

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Mol	Chain	Res	Type
2	B	357	MET
2	B	358	ARG
2	B	363	ASN
2	B	368	LEU
2	B	424	LYS
2	B	425	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	91	GLN
1	A	96	HIS
1	A	136	ASN
1	A	174	GLN
1	A	197	GLN
1	A	242	GLN
1	A	332	GLN
1	A	336	GLN
1	A	394	GLN
1	A	474	ASN
2	B	57	ASN
2	B	85	GLN
2	B	151	GLN
2	B	242	GLN
2	B	361	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CSD	A	280	1	3,7,8	0.82	0	1,8,10	3.08	1 (100%)

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	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	280	CSD	OD1-SG-CB	3.08	111.41	105.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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
4	UC1	A	999	-	19,23,23	1.85	3 (15%)	21,31,31	1.32	2 (9%)
3	PO4	A	1003	-	4,4,4	1.77	2 (50%)	6,6,6	0.35	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
4	UC1	A	999	-	-	2/10/14/14	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	UC1	C-N	6.12	1.39	1.34
4	A	999	UC1	CA-C8	3.38	1.53	1.48
3	A	1003	PO4	P-O2	-2.18	1.48	1.54
3	A	1003	PO4	P-O4	-2.08	1.48	1.54
4	A	999	UC1	C10-C9	2.02	1.51	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	UC1	S-C-N	-3.95	117.59	125.23
4	A	999	UC1	OB-C3-C4	3.02	120.13	116.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

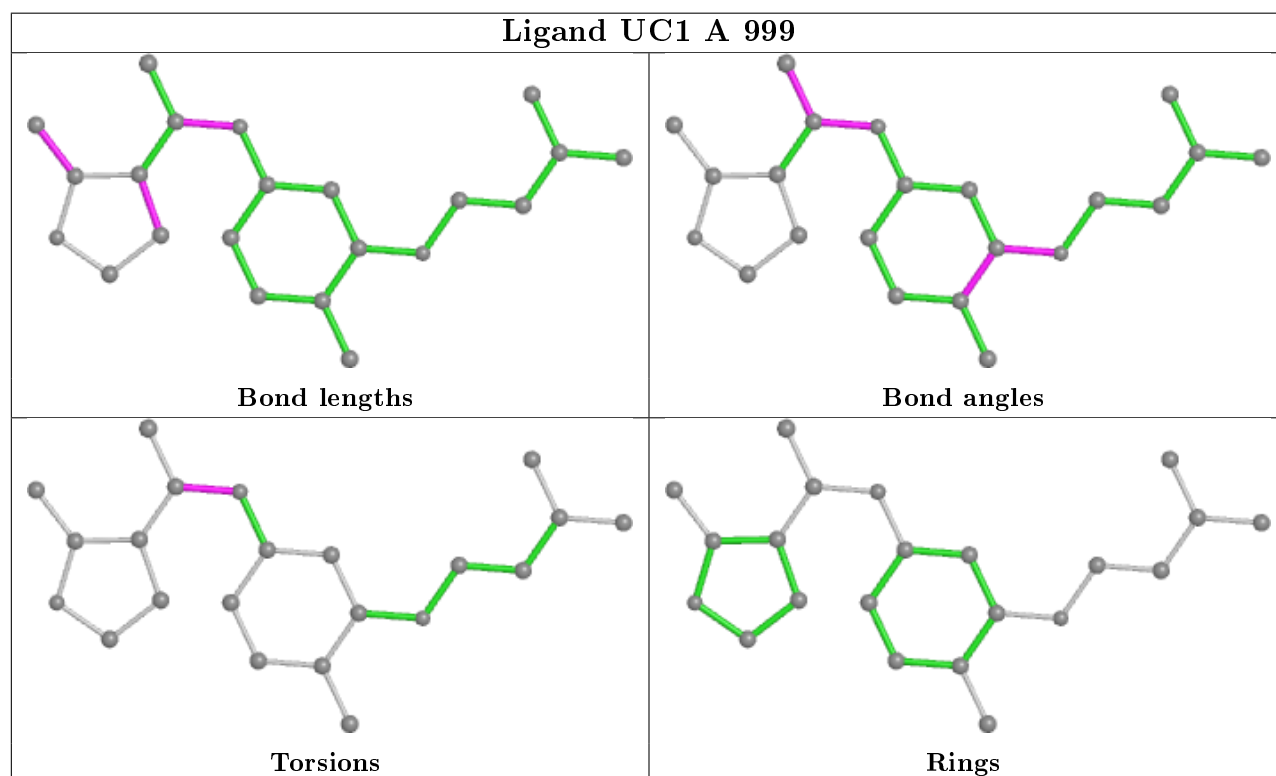
Mol	Chain	Res	Type	Atoms
4	A	999	UC1	C9-C-N-C1
4	A	999	UC1	S-C-N-C1

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	UC1	7	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	536/560 (95%)	0.01	39 (7%)	15 11	10, 57, 126, 182	0
2	B	404/440 (91%)	-0.17	10 (2%)	57 55	11, 50, 112, 155	0
All	All	940/1000 (94%)	-0.06	49 (5%)	27 23	10, 53, 119, 182	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	ASN	6.0
1	A	135	ILE	4.8
2	B	5	ILE	4.8
1	A	29	GLU	4.7
1	A	134	SER	4.5
1	A	28	GLU	4.4
1	A	52	PRO	4.3
1	A	1	PRO	4.0
1	A	90	VAL	3.9
1	A	67	ASP	3.9
1	A	63	ILE	3.8
1	A	91	GLN	3.6
1	A	30	LYS	3.6
1	A	33	ALA	3.4
1	A	68	SER	3.4
1	A	132	ILE	3.3
1	A	472	THR	3.3
1	A	542	ILE	3.3
1	A	245	VAL	3.3
1	A	55	PRO	3.3
2	B	433	PRO	3.3
2	B	67	ASP	3.2
2	B	432	GLU	3.1
1	A	27	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	3.1
2	B	6	GLU	3.0
1	A	74	LEU	2.8
1	A	450	THR	2.8
1	A	133	PRO	2.7
1	A	131	THR	2.7
2	B	198	HIS	2.6
1	A	473	THR	2.5
2	B	190	GLY	2.5
1	A	452	LEU	2.5
1	A	51	GLY	2.4
1	A	64	LYS	2.4
1	A	61	PHE	2.4
1	A	127	TYR	2.4
2	B	191	SER	2.3
1	A	62	ALA	2.3
1	A	21	VAL	2.3
1	A	65	LYS	2.3
2	B	242	GLN	2.3
1	A	448	ARG	2.2
1	A	69	THR	2.2
1	A	22	LYS	2.2
2	B	321	PRO	2.1
1	A	128	THR	2.1
1	A	25	PRO	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, 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
1	CSD	A	280	8/9	0.96	0.12	35,47,55,56	0

## 6.3 Carbohydrates [i](#)

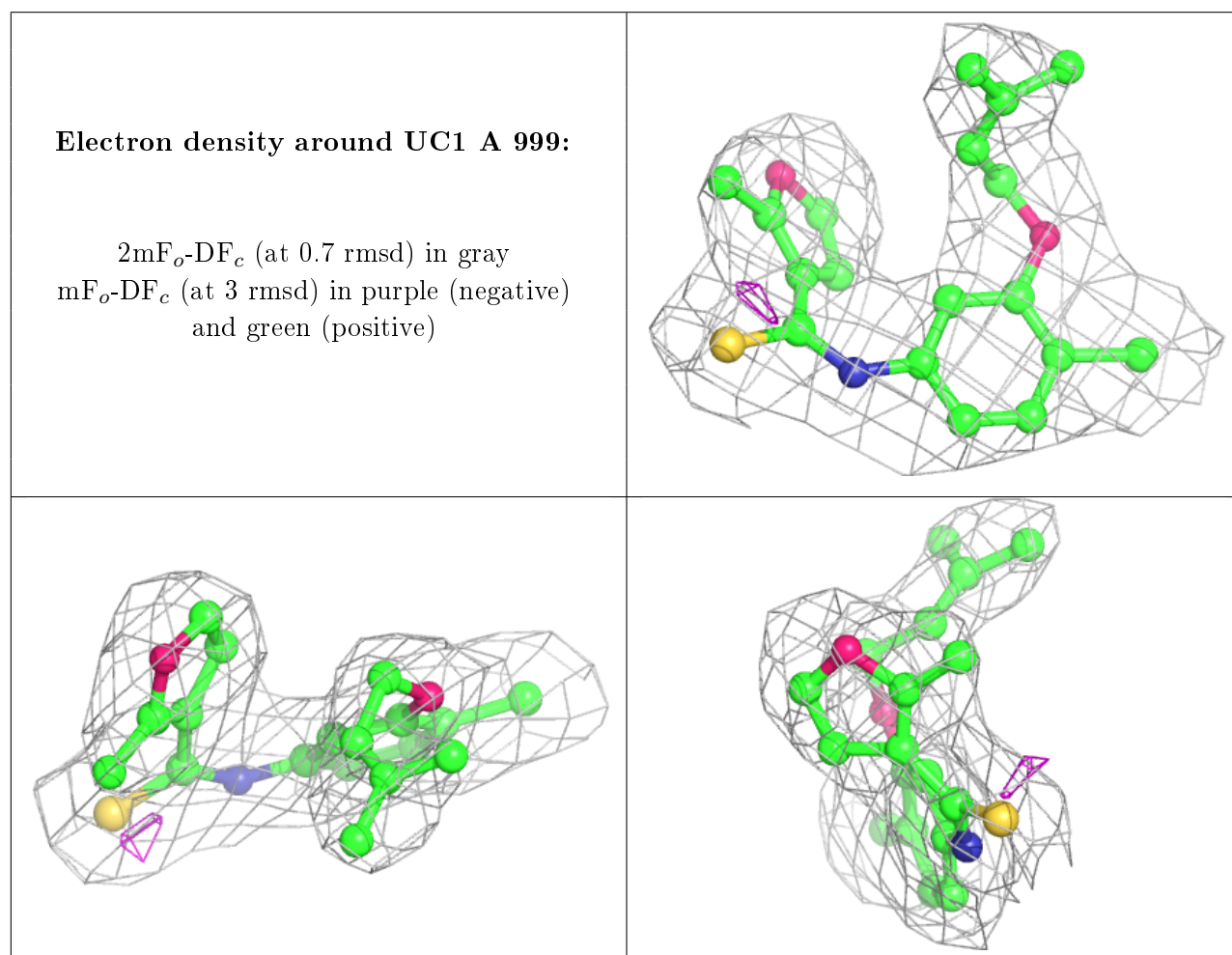
There are no carbohydrates in this entry.

## 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
3	PO4	A	1003	5/5	0.92	0.27	122,122,126,131	0
4	UC1	A	999	22/22	0.98	0.12	14,27,47,51	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.