



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:59 AM UTC

PDB ID : 2R9Q / pdb_00002r9q
Title : Crystal structure of 2'-deoxycytidine 5'-triphosphate deaminase from *Agrobacterium tumefaciens*
Authors : Zhang, R.; Dong, A.; Xu, X.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-09-13
Resolution : 2.20 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:

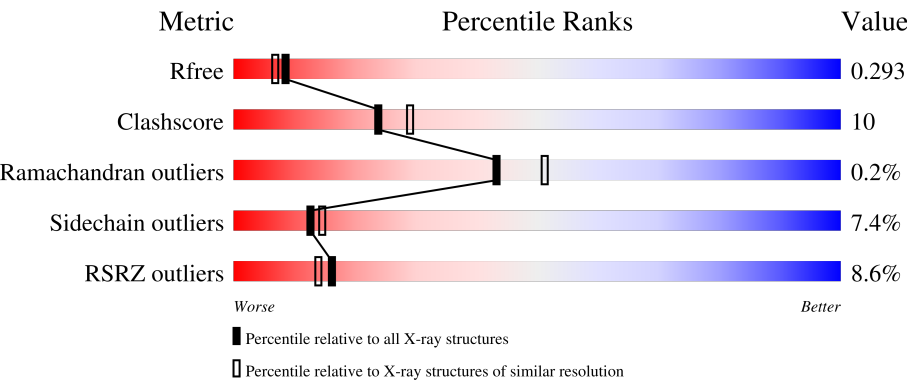
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	370	10% 70% 16% • 12%
1	B	370	5% 70% 19% • 8%
1	C	370	5% 69% 18% • 11%
1	D	370	8% 68% 19% • 11%
2	X	7	71% 57% 29% 14%

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Mol	Chain	Length	Quality of chain
3	Y	9	56% 56% 33% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10768 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 2'-deoxycytidine 5'-triphosphate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2478	1590	426	455	7			
1	B	342	Total	C	N	O	S	0	0	0
			2607	1664	456	480	7			
1	C	331	Total	C	N	O	S	0	0	0
			2493	1591	433	462	7			
1	D	330	Total	C	N	O	S	0	0	0
			2465	1584	425	449	7			

- Molecule 2 is a protein called Synthetic peptide 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	7	Total	C	N	O	S	0	0	0
			44	26	8	9	1			

- Molecule 3 is a protein called Synthetic peptide 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Y	9	Total	C	N	O	0	0	0
			59	39	9	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total	O	0	0
			152	152		
4	B	170	Total	O	0	0
			170	170		
4	C	138	Total	O	0	0
			138	138		
4	D	157	Total	O	0	0
			157	157		

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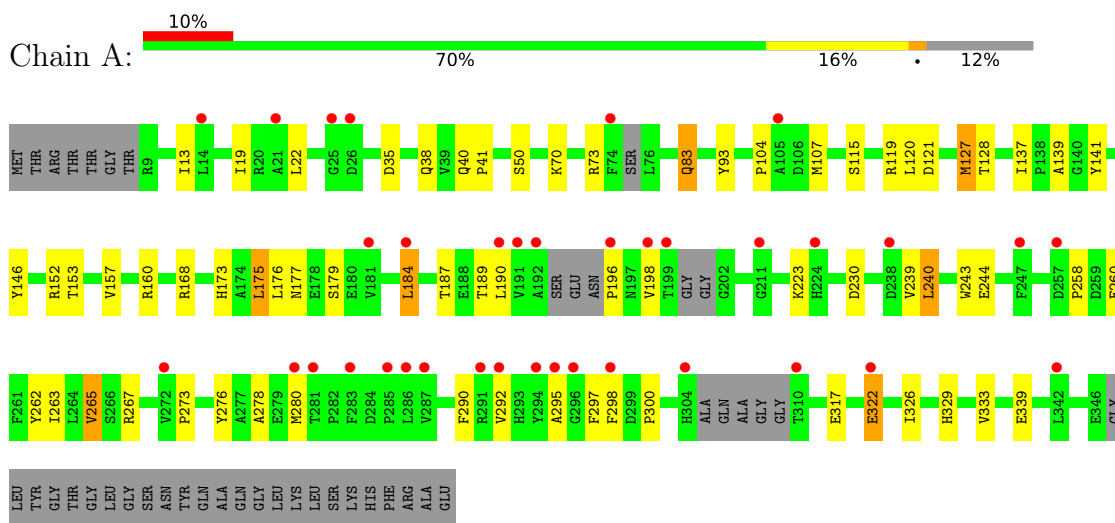
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	1	Total	O	0	0
			1	1		
4	Y	4	Total	O	0	0
			4	4		

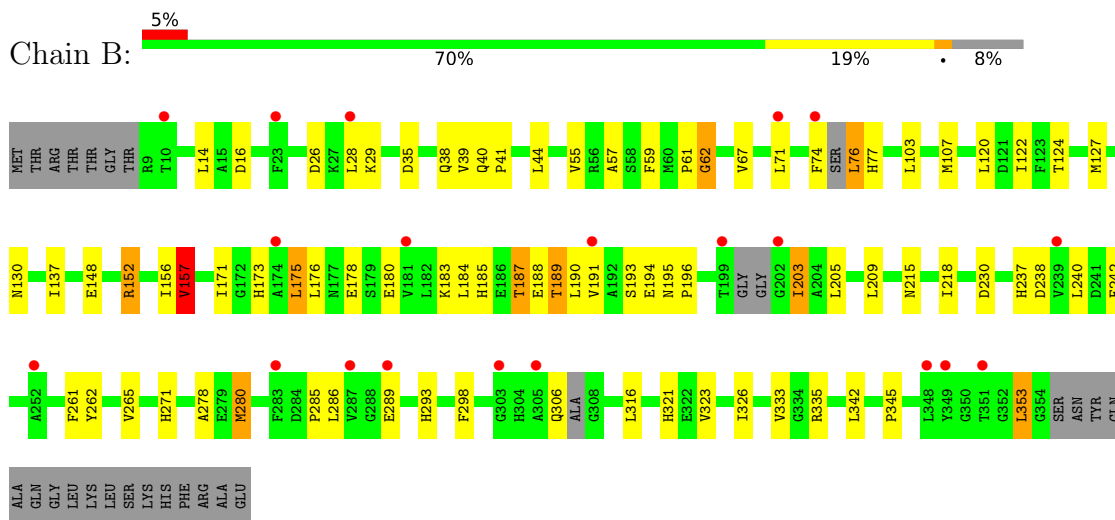
3 Residue-property plots

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: 2'-deoxycytidine 5'-triphosphate deaminase

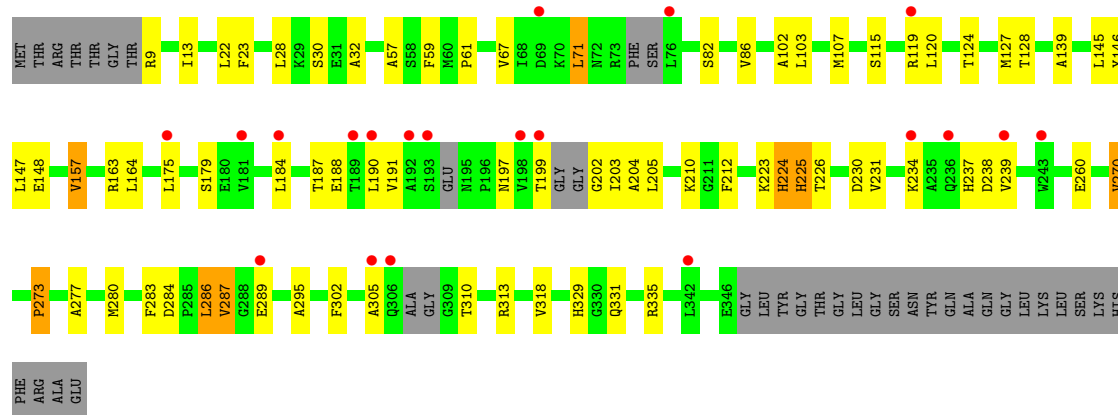


- Molecule 1: 2'-deoxycytidine 5'-triphosphate deaminase

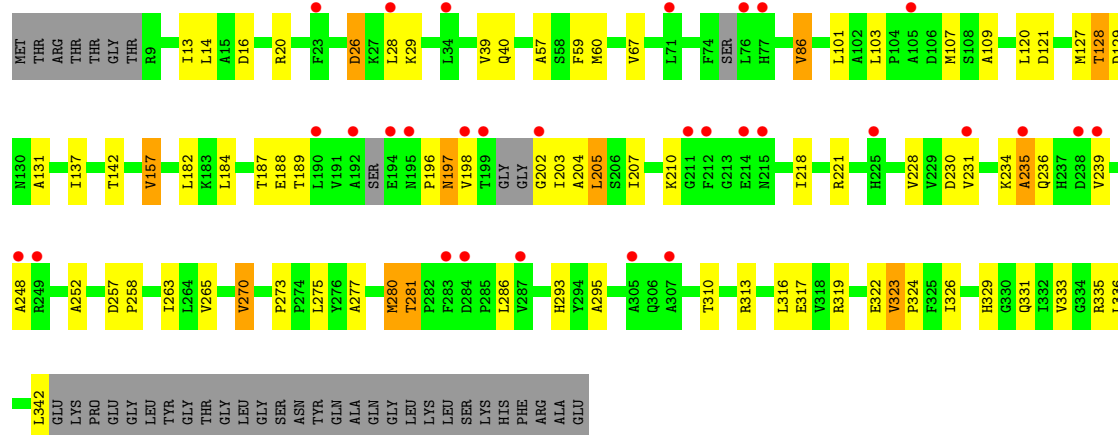


- Molecule 1: 2'-deoxycytidine 5'-triphosphate deaminase

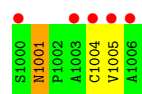




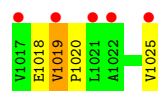
• Molecule 1: 2'-deoxycytidine 5'-triphosphate deaminase



• Molecule 2: Synthetic peptide 1



• Molecule 3: Synthetic peptide 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.69Å 129.04Å 85.56Å 90.00° 108.75° 90.00°	Depositor
Resolution (Å)	46.78 – 2.20 46.78 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.9 (46.78-2.20) 93.9 (46.78-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.269 0.218 , 0.293	Depositor DCC
R_{free} test set	690 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10768	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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

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	0.90	1/2531 (0.0%)	0.94	3/3434 (0.1%)
1	B	0.95	3/2663 (0.1%)	1.00	3/3609 (0.1%)
1	C	1.00	3/2545 (0.1%)	1.00	3/3457 (0.1%)
1	D	0.92	2/2520 (0.1%)	0.99	5/3428 (0.1%)
2	X	0.74	0/44	1.40	0/60
3	Y	0.93	0/59	0.86	0/81
All	All	0.94	9/10362 (0.1%)	0.99	14/14069 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	289	GLU	CB-CG	5.92	1.70	1.52
1	C	289	GLU	CA-C	5.72	1.58	1.52
1	B	218	ILE	CA-CB	5.67	1.62	1.54
1	B	157	VAL	CA-CB	5.49	1.60	1.54
1	C	102	ALA	CA-CB	5.31	1.58	1.53
1	D	333	VAL	CA-CB	5.20	1.60	1.54
1	D	86	VAL	CA-CB	5.19	1.60	1.54
1	A	93	TYR	C-O	-5.07	1.17	1.23
1	B	335	ARG	CA-C	5.02	1.58	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	239	VAL	N-CA-C	7.79	118.53	110.36
1	A	273	PRO	CA-C-N	6.99	128.58	119.84
1	A	273	PRO	C-N-CA	6.99	128.58	119.84
1	B	62	GLY	CA-C-N	6.44	126.79	119.83
1	B	62	GLY	C-N-CA	6.44	126.79	119.83
1	C	273	PRO	CA-C-N	6.14	125.84	119.82
1	C	273	PRO	C-N-CA	6.14	125.84	119.82
1	D	273	PRO	CA-C-N	6.11	127.47	119.84
1	D	273	PRO	C-N-CA	6.11	127.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	PRO	N-CA-C	5.79	121.58	113.53
1	D	273	PRO	O-C-N	5.61	123.89	121.31
1	D	26	ASP	N-CA-C	5.59	119.28	111.90
1	C	273	PRO	O-C-N	5.37	123.67	121.15
1	B	335	ARG	CB-CA-C	5.16	118.09	110.14

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	2478	0	2427	47	0
1	B	2607	0	2571	53	0
1	C	2493	0	2427	54	0
1	D	2465	0	2388	52	0
2	X	44	0	41	2	0
3	Y	59	0	63	1	0
4	A	152	0	0	2	0
4	B	170	0	0	2	0
4	C	138	0	0	9	0
4	D	157	0	0	8	0
4	X	1	0	0	0	0
4	Y	4	0	0	0	0
All	All	10768	0	9917	203	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 10.

All (203) 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:B:205:LEU:HD12	1:B:280:MET:HE3	1.22	1.13
1:A:260:GLU:OE1	1:A:262:TYR:OH	1.80	0.99
1:C:184:LEU:HD22	1:C:190:LEU:HD21	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:GLU:OE2	1:D:60:MET:HE2	1.74	0.88
1:B:205:LEU:HD12	1:B:280:MET:CE	2.06	0.83
1:B:286:LEU:HD22	1:B:289:GLU:OE1	1.77	0.82
1:D:128:THR:HG22	1:D:131:ALA:HB2	1.59	0.82
1:B:205:LEU:CD1	1:B:280:MET:HE3	2.07	0.82
1:C:184:LEU:HD21	1:C:273:PRO:HG2	1.63	0.80
1:B:152:ARG:HD3	1:D:322:GLU:OE1	1.83	0.79
1:B:289:GLU:HG3	4:D:382:HOH:O	1.84	0.78
1:C:287:VAL:HG12	4:C:504:HOH:O	1.82	0.78
1:A:322:GLU:N	4:A:523:HOH:O	2.06	0.75
1:B:173:HIS:CE1	1:B:175:LEU:HD21	2.21	0.75
1:C:184:LEU:CD2	1:C:190:LEU:HD21	2.18	0.73
1:A:243:TRP:CH2	1:A:263:ILE:HD11	2.25	0.72
1:B:152:ARG:HH11	1:B:152:ARG:HG3	1.53	0.71
1:A:22:LEU:HD21	1:A:107:MET:HE1	1.72	0.71
1:B:171:ILE:HD12	1:B:342:LEU:HD11	1.71	0.71
1:C:157:VAL:HG13	1:C:230:ASP:HA	1.72	0.71
1:C:67:VAL:HG12	1:C:71:LEU:CD2	2.22	0.70
1:A:223:LYS:HE3	1:A:244:GLU:HG3	1.75	0.68
1:C:199:THR:HG22	4:C:437:HOH:O	1.95	0.67
1:D:157:VAL:HG13	1:D:230:ASP:HA	1.78	0.66
1:D:205:LEU:HD23	1:D:280:MET:HE2	1.77	0.66
1:C:210:LYS:HG2	1:C:329:HIS:CE1	2.32	0.65
1:D:14:LEU:HD21	1:D:107:MET:CE	2.26	0.65
1:A:196:PRO:O	1:A:198:VAL:HG23	1.97	0.65
1:B:195:ASN:HB2	1:B:196:PRO:HD2	1.78	0.65
1:D:205:LEU:CD2	1:D:280:MET:HE2	2.27	0.64
1:D:280:MET:HB3	1:D:295:ALA:HB1	1.80	0.64
1:B:77:HIS:HB2	4:B:495:HOH:O	1.95	0.64
1:C:191:VAL:CG2	1:C:203:ILE:HD12	2.28	0.64
1:D:197:ASN:HB3	1:D:204:ALA:HB3	1.81	0.63
3:Y:1019:VAL:HG13	3:Y:1020:PRO:HD2	1.81	0.62
1:D:263:ILE:HD13	1:D:317:GLU:HG3	1.81	0.62
1:A:184:LEU:HD13	1:A:190:LEU:HD21	1.81	0.62
1:C:184:LEU:HD22	1:C:190:LEU:CD2	2.24	0.61
1:B:289:GLU:OE2	1:D:60:MET:CE	2.48	0.61
1:B:262:TYR:OH	4:B:541:HOH:O	2.12	0.60
1:B:61:PRO:HG3	1:B:127:MET:HE3	1.83	0.60
1:B:157:VAL:HG13	1:B:230:ASP:HA	1.84	0.58
1:A:127:MET:HG3	1:A:146:TYR:HB2	1.84	0.58
1:D:14:LEU:HD21	1:D:107:MET:HE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:PRO:HB2	1:D:203:ILE:HD12	1.86	0.58
1:B:183:LYS:O	1:B:187:THR:HG22	2.02	0.58
1:A:83:GLN:HA	1:A:83:GLN:HE21	1.67	0.57
1:D:207:ILE:HD12	4:D:525:HOH:O	2.04	0.57
1:A:177:ASN:OD1	1:A:179:SER:HB3	2.04	0.57
1:D:218:ILE:HD13	1:D:248:ALA:N	2.19	0.57
1:D:316:LEU:HD12	4:D:525:HOH:O	2.04	0.57
1:B:345:PRO:HB2	1:B:353:LEU:HG	1.87	0.57
1:A:267:ARG:HD3	1:A:329:HIS:CE1	2.39	0.57
1:C:59:PHE:CE1	1:C:127:MET:HE1	2.40	0.57
1:B:28:LEU:HD21	1:B:44:LEU:HD22	1.87	0.56
1:B:152:ARG:HG3	1:B:152:ARG:NH1	2.20	0.56
1:D:67:VAL:HG13	1:D:127:MET:HE2	1.87	0.56
1:D:182:LEU:HG	1:D:198:VAL:HG21	1.87	0.56
1:D:202:GLY:N	4:D:406:HOH:O	2.39	0.56
1:A:119:ARG:HD3	1:A:317:GLU:OE2	2.06	0.56
1:A:239:VAL:HG23	1:A:240:LEU:HD13	1.88	0.55
1:B:326:ILE:HG13	1:D:57:ALA:HB3	1.89	0.55
1:A:157:VAL:HG13	1:A:230:ASP:HA	1.88	0.55
1:D:128:THR:HG23	1:D:129:ASP:O	2.06	0.55
1:C:13:ILE:HD13	1:C:277:ALA:HB3	1.89	0.55
1:B:293:HIS:NE2	1:B:321:HIS:CE1	2.75	0.55
1:D:121:ASP:OD2	1:D:319:ARG:NH2	2.39	0.54
1:C:67:VAL:HG12	1:C:71:LEU:HD23	1.90	0.54
1:A:173:HIS:CE1	1:A:175:LEU:HD21	2.42	0.54
1:A:290:PHE:CE2	1:A:333:VAL:HG12	2.43	0.54
1:C:107:MET:O	1:C:139:ALA:HA	2.08	0.53
1:C:128:THR:HG22	1:C:145:LEU:HD23	1.89	0.53
1:C:13:ILE:CD1	1:C:277:ALA:HB3	2.39	0.53
1:C:61:PRO:HG3	1:C:127:MET:CE	2.39	0.52
1:D:270:VAL:HG11	1:D:336:LEU:HD22	1.91	0.52
1:A:13:ILE:HD13	1:A:168:ARG:HD3	1.90	0.52
1:A:128:THR:HG21	1:A:137:ILE:HG13	1.91	0.52
1:A:243:TRP:CH2	1:A:263:ILE:CD1	2.91	0.52
1:C:124:THR:HA	1:C:148:GLU:O	2.10	0.52
1:C:61:PRO:HG3	1:C:127:MET:HE3	1.91	0.51
1:C:212:PHE:HE2	1:C:313:ARG:HH12	1.59	0.51
1:B:185:HIS:O	1:B:188:GLU:O	2.29	0.51
1:A:326:ILE:HG13	1:C:57:ALA:HB3	1.93	0.51
1:B:191:VAL:CG2	1:B:203:ILE:HD13	2.41	0.51
1:C:22:LEU:HD21	1:C:107:MET:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:PHE:CE2	1:C:286:LEU:HD12	2.45	0.51
1:B:184:LEU:HA	1:B:187:THR:CG2	2.40	0.51
1:D:280:MET:HE3	1:D:316:LEU:HD21	1.92	0.51
1:C:283:PHE:HE2	1:C:286:LEU:HD12	1.76	0.51
1:D:235:ALA:HB3	4:D:457:HOH:O	2.11	0.51
1:D:293:HIS:CE1	1:D:319:ARG:HB2	2.46	0.50
2:X:1001:ASN:C	2:X:1001:ASN:ND2	2.68	0.50
1:C:224:HIS:CD2	1:C:260:GLU:OE2	2.64	0.50
1:D:16:ASP:OD2	1:D:20:ARG:NH2	2.44	0.50
1:B:137:ILE:HD12	1:B:137:ILE:N	2.27	0.50
1:D:109:ALA:HB3	1:D:137:ILE:HB	1.94	0.50
1:D:316:LEU:HB2	4:D:525:HOH:O	2.12	0.50
1:D:265:VAL:CG2	1:D:313:ARG:HB3	2.42	0.50
1:C:237:HIS:NE2	4:C:500:HOH:O	2.27	0.49
1:C:115:SER:O	1:C:119:ARG:HG2	2.12	0.49
1:C:280:MET:O	1:C:295:ALA:HB1	2.11	0.49
1:B:316:LEU:HD13	1:B:333:VAL:HG21	1.94	0.49
1:A:176:LEU:HD21	1:A:276:TYR:CE1	2.48	0.49
1:A:243:TRP:CZ3	1:A:263:ILE:HD12	2.47	0.49
1:B:122:ILE:HD13	1:B:156:ILE:HD13	1.95	0.49
1:C:202:GLY:N	4:C:414:HOH:O	2.45	0.49
1:A:128:THR:HB	1:A:141:TYR:CZ	2.47	0.48
1:C:199:THR:CG2	1:C:335:ARG:HD2	2.42	0.48
1:A:184:LEU:O	1:A:184:LEU:HD22	2.14	0.48
1:B:55:VAL:HG12	1:B:76:LEU:CD2	2.44	0.48
1:A:19:ILE:HA	1:A:22:LEU:HD12	1.95	0.48
1:C:231:VAL:O	1:C:234:LYS:HE2	2.13	0.48
1:D:59:PHE:CE1	1:D:127:MET:HE1	2.48	0.48
1:A:40:GLN:HB3	1:A:41:PRO:HD2	1.96	0.48
1:A:280:MET:CE	1:A:292:VAL:HG11	2.44	0.48
1:C:226:THR:N	4:C:495:HOH:O	2.45	0.47
1:D:13:ILE:HD12	1:D:277:ALA:HB3	1.96	0.47
1:C:61:PRO:CG	1:C:127:MET:HE3	2.43	0.47
1:C:124:THR:HB	1:C:147:LEU:HD11	1.95	0.47
1:A:121:ASP:OD2	1:A:153:THR:OG1	2.25	0.47
1:D:280:MET:HE3	1:D:316:LEU:CD2	2.44	0.47
1:D:16:ASP:HB3	1:D:40:GLN:O	2.15	0.47
1:A:137:ILE:HD12	1:A:137:ILE:N	2.29	0.47
1:D:67:VAL:CG1	1:D:127:MET:HE2	2.46	0.46
1:B:67:VAL:HG13	1:B:127:MET:HE2	1.97	0.46
1:D:207:ILE:CD1	4:D:525:HOH:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:MET:O	1:A:295:ALA:HB1	2.15	0.46
1:A:265:VAL:HG22	4:A:519:HOH:O	2.15	0.46
1:C:23:PHE:HB2	1:C:28:LEU:HD23	1.97	0.46
1:A:121:ASP:O	1:A:152:ARG:HB2	2.16	0.46
1:C:184:LEU:HD21	1:C:273:PRO:CG	2.42	0.46
1:B:61:PRO:HG3	1:B:127:MET:CE	2.46	0.46
1:C:9:ARG:N	4:C:388:HOH:O	2.49	0.45
1:A:223:LYS:HE3	1:A:244:GLU:CG	2.45	0.45
1:A:176:LEU:HD12	1:A:176:LEU:N	2.31	0.45
1:D:16:ASP:HB2	1:D:39:VAL:HG12	1.97	0.45
1:D:184:LEU:O	1:D:188:GLU:O	2.34	0.45
1:D:221:ARG:NH1	4:D:518:HOH:O	2.49	0.45
1:B:293:HIS:NE2	1:B:321:HIS:HE1	2.14	0.45
1:B:124:THR:HA	1:B:148:GLU:O	2.16	0.45
1:D:189:THR:HB	1:D:310:THR:HG21	1.99	0.45
1:D:323:VAL:HG12	1:D:324:PRO:O	2.17	0.45
1:A:107:MET:O	1:A:139:ALA:HA	2.17	0.44
1:B:62:GLY:O	1:B:130:ASN:HA	2.17	0.44
1:D:205:LEU:HD23	1:D:280:MET:CE	2.47	0.44
1:A:128:THR:CG2	1:A:137:ILE:HG13	2.47	0.44
1:C:163:ARG:C	1:C:164:LEU:HD12	2.42	0.44
1:A:50:SER:OG	1:A:160:ARG:HD2	2.18	0.44
1:B:35:ASP:HB2	1:B:38:GLN:HB2	2.00	0.44
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.83	0.44
1:C:184:LEU:O	1:C:188:GLU:O	2.35	0.44
2:X:1001:ASN:C	2:X:1001:ASN:HD22	2.23	0.44
1:B:74:PHE:CB	1:B:76:LEU:HD23	2.48	0.44
1:C:270:VAL:HG12	1:C:302:PHE:CE2	2.53	0.43
1:A:115:SER:O	1:A:119:ARG:HG2	2.18	0.43
1:A:243:TRP:CZ3	1:A:263:ILE:CD1	3.02	0.43
1:B:185:HIS:HD2	1:B:190:LEU:H	1.66	0.43
1:A:157:VAL:CG1	1:A:230:ASP:HA	2.48	0.43
1:C:270:VAL:HG12	1:C:302:PHE:HE2	1.83	0.43
1:C:199:THR:HG23	1:C:335:ARG:HD2	1.99	0.43
1:D:286:LEU:HD12	1:D:331:GLN:NE2	2.33	0.43
1:D:234:LYS:C	1:D:236:GLN:H	2.27	0.43
1:A:13:ILE:HD11	1:A:339:GLU:CD	2.44	0.43
1:B:16:ASP:HB3	1:B:39:VAL:HG12	2.00	0.43
1:B:55:VAL:HG12	1:B:76:LEU:HD21	2.01	0.43
1:C:164:LEU:HD12	1:C:164:LEU:N	2.34	0.42
1:D:14:LEU:HD21	1:D:107:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASP:HB2	1:A:38:GLN:HB2	2.00	0.42
1:B:57:ALA:HB3	1:D:326:ILE:HG13	2.01	0.42
1:C:86:VAL:HG12	4:C:384:HOH:O	2.20	0.42
1:A:168:ARG:NH2	1:A:297:PHE:HB3	2.34	0.42
1:C:127:MET:HG3	1:C:146:TYR:HB2	2.02	0.42
1:C:305:ALA:HB2	1:C:310:THR:OG1	2.19	0.42
1:A:70:LYS:O	1:A:73:ARG:HB3	2.20	0.42
1:B:61:PRO:CG	1:B:127:MET:HE3	2.49	0.42
1:B:173:HIS:CE1	1:B:175:LEU:CD2	2.99	0.42
1:B:14:LEU:HD21	1:B:107:MET:CE	2.50	0.41
1:D:205:LEU:HD22	1:D:280:MET:HE2	1.99	0.41
1:B:194:GLU:HA	1:B:195:ASN:HA	1.72	0.41
1:D:101:LEU:O	1:D:142:THR:HA	2.20	0.41
1:C:30:SER:HB3	1:C:32:ALA:O	2.20	0.41
1:C:119:ARG:HB3	4:C:486:HOH:O	2.19	0.41
1:B:40:GLN:HB3	1:B:41:PRO:HD2	2.03	0.41
1:B:237:HIS:HB3	1:B:242:PHE:CE2	2.55	0.41
1:D:281:THR:HG22	1:D:335:ARG:CG	2.51	0.41
1:A:278:ALA:HB3	1:A:298:PHE:HB2	2.03	0.41
1:D:252:ALA:HB1	1:D:329:HIS:HB2	2.01	0.41
1:B:193:SER:O	1:B:195:ASN:HA	2.21	0.41
1:B:59:PHE:CE1	1:B:127:MET:HE1	2.55	0.41
1:C:67:VAL:HG22	1:C:127:MET:HE2	2.01	0.41
1:C:197:ASN:HB3	1:C:204:ALA:HB3	2.02	0.41
1:C:286:LEU:HD13	1:C:331:GLN:NE2	2.36	0.41
1:A:104:PRO:HG2	1:A:107:MET:HE3	2.02	0.41
1:B:189:THR:O	1:B:271:HIS:HD2	2.04	0.41
1:B:278:ALA:HB3	1:B:298:PHE:HB2	2.03	0.40
1:C:184:LEU:O	1:C:184:LEU:HD23	2.20	0.40
1:C:210:LYS:HE3	1:C:329:HIS:CD2	2.55	0.40
1:D:257:ASP:HA	1:D:258:PRO:HD3	1.96	0.40
1:B:176:LEU:HD12	1:B:176:LEU:N	2.36	0.40
1:A:276:TYR:O	1:A:300:PRO:HB3	2.21	0.40
1:B:74:PHE:HB2	1:B:76:LEU:HD23	2.03	0.40
1:B:285:PRO:O	1:B:286:LEU:HD23	2.21	0.40
1:C:225:HIS:CD2	4:C:501:HOH:O	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	317/370 (86%)	309 (98%)	7 (2%)	1 (0%)	36	42
1	B	334/370 (90%)	325 (97%)	9 (3%)	0	100	100
1	C	321/370 (87%)	308 (96%)	13 (4%)	0	100	100
1	D	322/370 (87%)	311 (97%)	10 (3%)	1 (0%)	36	42
2	X	5/7 (71%)	5 (100%)	0	0	100	100
3	Y	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1306/1496 (87%)	1264 (97%)	40 (3%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	GLU
1	D	235	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	254/302 (84%)	245 (96%)	9 (4%)	32	43
1	B	270/302 (89%)	246 (91%)	24 (9%)	9	10
1	C	255/302 (84%)	236 (92%)	19 (8%)	12	14
1	D	246/302 (82%)	227 (92%)	19 (8%)	12	13
2	X	5/5 (100%)	2 (40%)	3 (60%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Y	6/6 (100%)	3 (50%)	3 (50%)	0	0
All	All	1036/1219 (85%)	959 (93%)	77 (7%)	13	14

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	120	LEU
1	A	127	MET
1	A	175	LEU
1	A	184	LEU
1	A	187	THR
1	A	189	THR
1	A	240	LEU
1	A	265	VAL
1	B	26	ASP
1	B	29	LYS
1	B	71	LEU
1	B	76	LEU
1	B	103	LEU
1	B	120	LEU
1	B	152	ARG
1	B	157	VAL
1	B	175	LEU
1	B	178	GLU
1	B	180	GLU
1	B	187	THR
1	B	189	THR
1	B	203	ILE
1	B	209	LEU
1	B	215	ASN
1	B	238	ASP
1	B	240	LEU
1	B	261	PHE
1	B	265	VAL
1	B	280	MET
1	B	306	GLN
1	B	323	VAL
1	B	353	LEU
1	C	71	LEU
1	C	82	SER
1	C	103	LEU

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Mol	Chain	Res	Type
1	C	120	LEU
1	C	157	VAL
1	C	175	LEU
1	C	179	SER
1	C	187	THR
1	C	205	LEU
1	C	223	LYS
1	C	224	HIS
1	C	225	HIS
1	C	238	ASP
1	C	239	VAL
1	C	270	VAL
1	C	284	ASP
1	C	286	LEU
1	C	287	VAL
1	C	318	VAL
1	D	26	ASP
1	D	28	LEU
1	D	29	LYS
1	D	86	VAL
1	D	103	LEU
1	D	120	LEU
1	D	128	THR
1	D	157	VAL
1	D	187	THR
1	D	197	ASN
1	D	205	LEU
1	D	210	LYS
1	D	228	VAL
1	D	231	VAL
1	D	270	VAL
1	D	275	LEU
1	D	280	MET
1	D	281	THR
1	D	323	VAL
2	X	1001	ASN
2	X	1004	CYS
2	X	1005	VAL
3	Y	1018	GLU
3	Y	1019	VAL
3	Y	1025	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	173	HIS
1	A	236	GLN
1	B	77	HIS
1	B	132	GLN
1	B	166	GLN
1	B	173	HIS
1	B	185	HIS
1	B	215	ASN
1	B	271	HIS
1	B	321	HIS
1	B	331	GLN
1	C	225	HIS
1	C	237	HIS
1	C	331	GLN
1	C	340	HIS
1	D	130	ASN
1	D	173	HIS
1	D	197	ASN
1	D	331	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	327/370 (88%)	0.96	36 (11%) 10 8	48, 74, 103, 107	0
1	B	342/370 (92%)	0.72	20 (5%) 29 25	48, 68, 92, 106	0
1	C	331/370 (89%)	0.76	20 (6%) 27 24	51, 68, 97, 109	0
1	D	330/370 (89%)	0.99	30 (9%) 15 12	52, 75, 97, 118	0
2	X	7/7 (100%)	2.44	5 (71%) 0 0	93, 93, 100, 102	0
3	Y	9/9 (100%)	1.98	5 (55%) 0 0	84, 86, 88, 88	0
All	All	1346/1496 (89%)	0.87	116 (8%) 16 14	48, 71, 99, 118	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	PRO	4.4
1	D	28	LEU	4.4
1	C	76	LEU	4.3
1	D	215	ASN	4.2
1	D	76	LEU	4.1
1	A	285	PRO	3.7
1	A	25	GLY	3.5
1	B	202	GLY	3.5
1	C	198	VAL	3.4
1	D	23	PHE	3.3
3	Y	1025	VAL	3.3
3	Y	1017	VAL	3.3
1	D	195	ASN	3.1
1	B	349	TYR	3.1
1	B	348	LEU	3.1
1	C	199	THR	3.1
1	A	199	THR	3.1
1	C	305	ALA	3.1
1	A	247	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	305	ALA	3.0
1	A	190	LEU	3.0
1	B	287	VAL	3.0
1	B	199	THR	3.0
1	B	28	LEU	2.9
1	A	14	LEU	2.9
1	A	286	LEU	2.9
1	D	105	ALA	2.9
1	A	304	HIS	2.9
1	D	194	GLU	2.9
1	D	211	GLY	2.9
1	B	181	VAL	2.9
1	D	199	THR	2.9
2	X	1006	ALA	2.8
1	A	292	VAL	2.8
2	X	1004	CYS	2.8
1	B	289	GLU	2.8
2	X	1003	ALA	2.8
1	C	289	GLU	2.8
3	Y	1021	LEU	2.7
1	A	211	GLY	2.7
2	X	1000	SER	2.7
1	A	283	PHE	2.7
1	B	74	PHE	2.7
1	B	239	VAL	2.7
1	B	351	THR	2.7
1	A	105	ALA	2.6
1	B	305	ALA	2.6
1	A	192	ALA	2.6
1	C	239	VAL	2.6
1	A	294	TYR	2.6
1	C	234	LYS	2.6
1	D	71	LEU	2.5
1	D	235	ALA	2.5
1	C	243	TRP	2.5
1	A	310	THR	2.5
1	D	283	PHE	2.5
1	A	184	LEU	2.5
1	A	238	ASP	2.5
1	D	192	ALA	2.5
1	B	23	PHE	2.5
1	C	181	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	193	SER	2.5
1	D	287	VAL	2.5
1	A	224	HIS	2.4
1	D	77	HIS	2.4
1	C	192	ALA	2.4
1	A	287	VAL	2.4
1	D	212	PHE	2.4
1	C	236	GLN	2.4
1	C	306	GLN	2.4
1	D	202	GLY	2.4
1	A	198	VAL	2.4
1	B	71	LEU	2.4
1	A	26	ASP	2.4
1	D	284	ASP	2.4
1	A	342	LEU	2.4
1	D	248	ALA	2.3
1	A	74	PHE	2.3
1	A	322	GLU	2.3
1	B	283	PHE	2.3
1	C	342	LEU	2.3
1	A	257	ASP	2.3
1	D	238	ASP	2.3
1	C	189	THR	2.3
1	B	303	GLY	2.3
1	C	190	LEU	2.2
3	Y	1019	VAL	2.3
1	C	69	ASP	2.2
1	D	225	HIS	2.2
1	A	181	VAL	2.2
1	D	198	VAL	2.2
1	D	249	ARG	2.2
1	A	296	GLY	2.2
1	B	191	VAL	2.2
1	A	191	VAL	2.2
1	A	280	MET	2.2
1	A	295	ALA	2.2
1	A	291	ARG	2.1
1	D	34	LEU	2.1
1	D	214	GLU	2.1
1	B	10	THR	2.1
2	X	1005	VAL	2.1
1	A	281	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	174	ALA	2.1
1	B	252	ALA	2.1
1	D	307	ALA	2.1
3	Y	1022	ALA	2.1
1	D	190	LEU	2.1
1	A	298	PHE	2.1
1	C	184	LEU	2.0
1	A	272	VAL	2.0
1	C	119	ARG	2.0
1	D	231	VAL	2.0
1	D	239	VAL	2.0
1	A	21	ALA	2.0
1	C	175	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.