



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 04:10 PM JST

PDB ID : 8K1I
Title : Crystal structure of arabinose dehydrogenase from *Candida auris*
Authors : Zhang, J.; Bai, X.; He, S.R.; Zhao, Z.D.
Deposited on : 2023-07-11
Resolution : 1.95 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

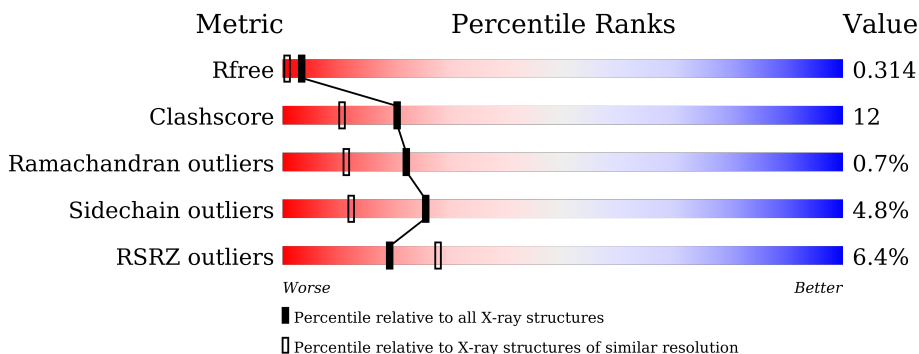
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	351	 6% 75% 22% ..
1	B	351	 9% 65% 32% ..
1	C	351	 5% 69% 29% ..
1	D	351	 5% 71% 23% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11511 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 NADP-dependent oxidoreductase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	Total 2778	C 1787	N 458	O 525	S 8	0	0	0
1	B	348	Total 2788	C 1793	N 460	O 526	S 9	0	0	0
1	C	346	Total 2767	C 1778	N 457	O 524	S 8	0	0	0
1	D	343	Total 2753	C 1772	N 452	O 520	S 9	0	0	0

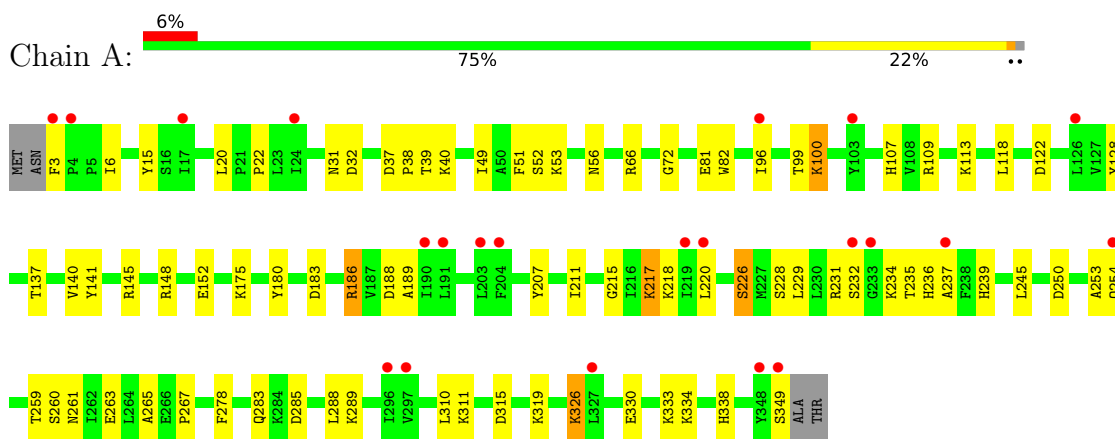
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	112	Total 112	O 112	0	0
2	B	99	Total 99	O 99	0	0
2	C	106	Total 106	O 106	0	0
2	D	108	Total 108	O 108	0	0

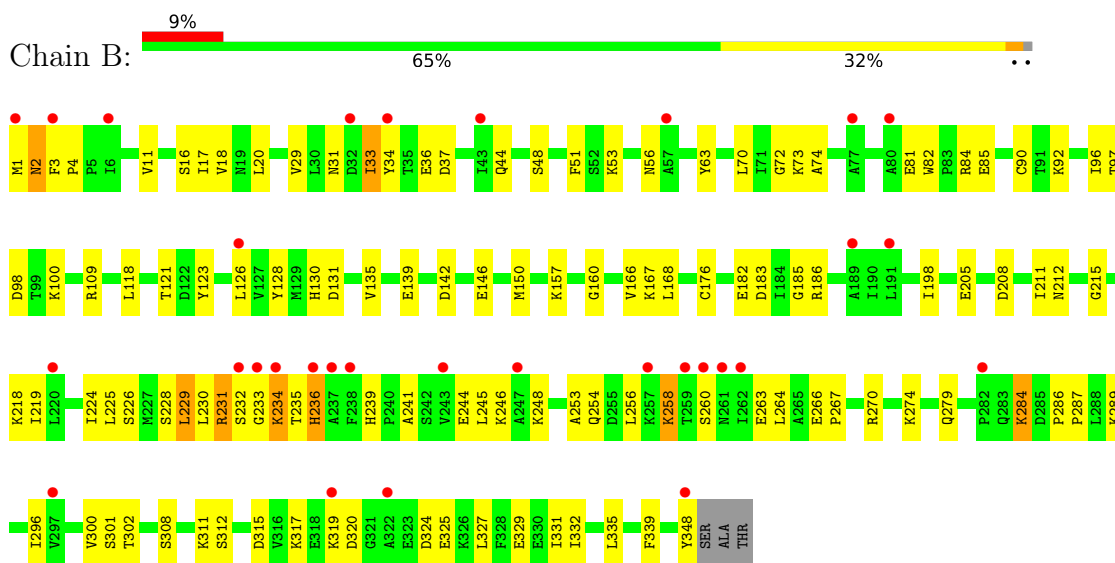
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NADP-dependent oxidoreductase domain-containing protein

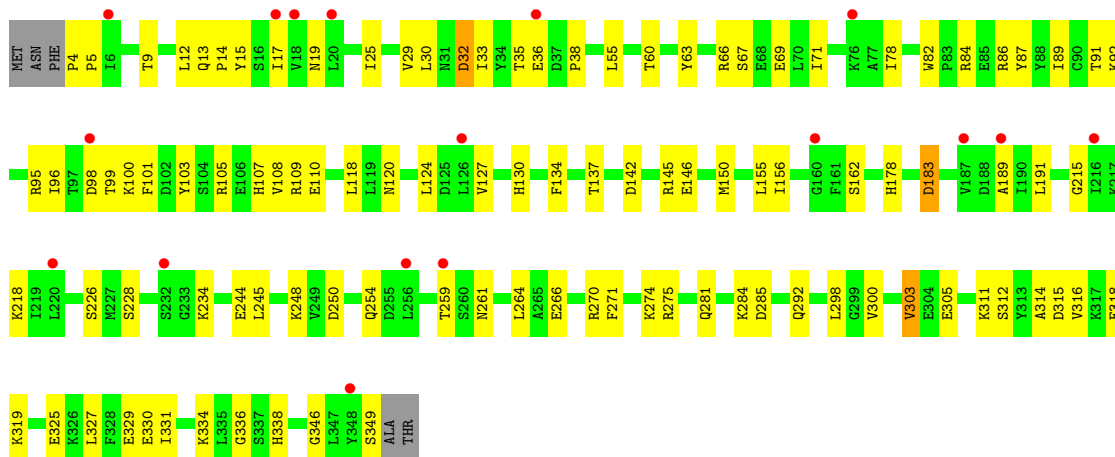


- Molecule 1: NADP-dependent oxidoreductase domain-containing protein

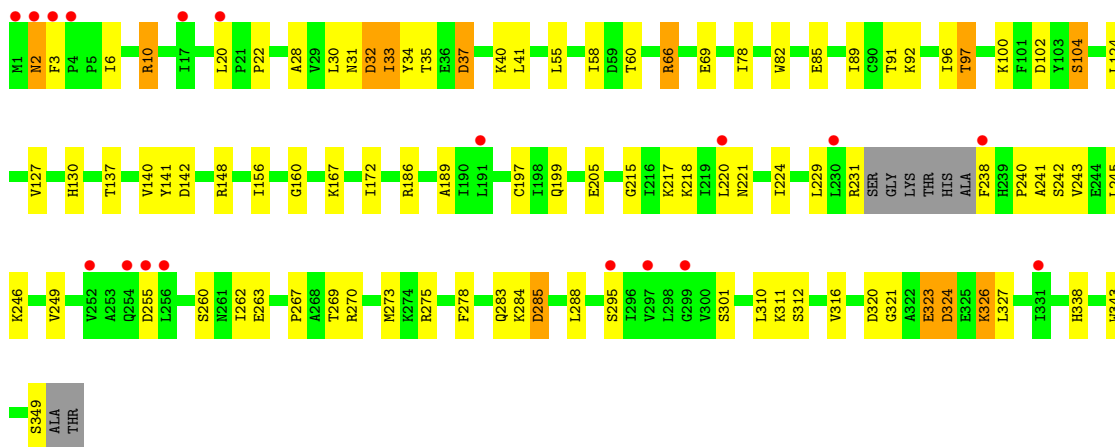


- Molecule 1: NADP-dependent oxidoreductase domain-containing protein





● Molecule 1: NADP-dependent oxidoreductase domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.63Å 91.12Å 227.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.64 – 1.95 34.30 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.64-1.95) 100.0 (34.30-1.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.95Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.255 , 0.314 0.255 , 0.314	Depositor DCC
R_{free} test set	5509 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11511	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.97% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/2841	0.66	2/3849 (0.1%)
1	B	0.44	0/2851	0.64	0/3862
1	C	0.47	0/2829	0.64	0/3832
1	D	0.44	0/2814	0.64	0/3811
All	All	0.46	0/11335	0.65	2/15354 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	PRO	N-CD-CG	-5.17	95.45	103.20
1	A	38	PRO	CA-N-CD	-5.05	104.42	111.50

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	2778	0	2789	60	1
1	B	2788	0	2802	82	0
1	C	2767	0	2781	72	0
1	D	2753	0	2766	68	1
2	A	112	0	0	12	0
2	B	99	0	0	13	0
2	C	106	0	0	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	108	0	0	16	0
All	All	11511	0	11138	275	1

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 (275) 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:D:221:ASN:ND2	2:D:402:HOH:O	2.04	0.90
1:B:109:ARG:NH2	1:B:146:GLU:OE2	2.12	0.81
1:D:97:THR:HG23	1:D:100:LYS:HB2	1.63	0.80
1:C:259:THR:N	2:C:405:HOH:O	2.14	0.80
1:B:182:GLU:OE2	2:B:401:HOH:O	2.01	0.79
1:A:283:GLN:NE2	2:A:402:HOH:O	2.15	0.78
1:B:198:ILE:HG22	1:B:230:LEU:HD13	1.65	0.77
1:B:236:HIS:HE1	1:B:246:LYS:HG2	1.50	0.77
1:C:248:LYS:HG2	1:C:338:HIS:HD2	1.49	0.76
1:B:317:LYS:NZ	2:B:403:HOH:O	2.17	0.76
1:D:243:VAL:HA	1:D:246:LYS:HE2	1.67	0.76
1:C:13:GLN:HE22	1:C:15:TYR:HB2	1.49	0.76
1:A:330:GLU:OE1	2:A:401:HOH:O	2.04	0.75
1:D:283:GLN:OE1	2:D:401:HOH:O	2.03	0.75
1:B:232:SER:OG	1:B:263:GLU:OE1	2.05	0.75
1:B:1:MET:O	1:B:53:LYS:NZ	2.20	0.73
1:B:121:THR:HG22	1:B:123:TYR:H	1.53	0.73
1:B:100:LYS:O	2:B:402:HOH:O	2.07	0.72
1:A:145:ARG:NH1	1:A:183:ASP:OD2	2.22	0.72
1:A:289:LYS:N	2:A:402:HOH:O	2.21	0.72
1:D:197:CYS:SG	2:D:501:HOH:O	2.48	0.71
1:C:330:GLU:OE2	2:C:401:HOH:O	2.06	0.71
1:B:236:HIS:CE1	1:B:246:LYS:HG2	2.26	0.71
1:D:326:LYS:NZ	2:D:408:HOH:O	2.23	0.70
1:B:274:LYS:O	1:B:279:GLN:HG3	1.91	0.70
1:A:186:ARG:HD2	1:A:215:GLY:HA3	1.72	0.70
1:D:323:GLU:HA	1:D:326:LYS:HG2	1.73	0.70
1:D:311:LYS:NZ	2:D:410:HOH:O	2.23	0.70
1:C:69:GLU:OE2	2:C:402:HOH:O	2.10	0.69
1:B:85:GLU:OE1	1:B:85:GLU:N	2.18	0.68
1:B:186:ARG:HD2	1:B:215:GLY:HA3	1.74	0.68
1:B:224:ILE:HG21	1:B:296:ILE:HD13	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:HD1	2:A:402:HOH:O	1.77	0.68
1:D:55:LEU:HD11	1:D:310:LEU:HD21	1.76	0.68
1:C:305:GLU:O	2:C:404:HOH:O	2.13	0.67
1:C:315:ASP:OD2	2:C:403:HOH:O	2.12	0.67
1:A:188:ASP:OD1	1:A:217:LYS:HE3	1.95	0.67
1:B:234:LYS:HD3	1:B:235:THR:H	1.60	0.66
1:A:186:ARG:NH2	1:D:215:GLY:O	2.29	0.66
1:B:229:LEU:HD23	1:B:230:LEU:HD23	1.77	0.66
1:D:320:ASP:OD1	2:D:403:HOH:O	2.14	0.64
1:B:36:GLU:HG3	1:B:37:ASP:H	1.62	0.64
1:D:245:LEU:O	1:D:249:VAL:HG23	1.98	0.64
1:D:312:SER:OG	2:D:405:HOH:O	2.15	0.64
1:A:37:ASP:HB3	1:A:40:LYS:HG2	1.79	0.64
1:D:28:ALA:O	1:D:31:ASN:HB2	1.96	0.64
1:C:162:SER:HB3	1:C:191:LEU:HB3	1.79	0.64
1:C:275:ARG:HB2	2:C:407:HOH:O	1.96	0.64
1:A:96:ILE:HD11	1:A:107:HIS:CE1	2.33	0.64
1:D:186:ARG:HD2	1:D:215:GLY:HA3	1.79	0.63
1:A:330:GLU:O	1:A:334:LYS:HG3	1.98	0.63
1:C:33:ILE:HD12	1:C:33:ILE:H	1.63	0.63
1:C:12:LEU:HD22	1:C:12:LEU:H	1.64	0.62
1:D:58:ILE:HD11	1:D:89:ILE:HG23	1.82	0.62
1:A:3:PHE:N	2:A:411:HOH:O	2.33	0.62
1:B:31:ASN:HD22	1:B:33:ILE:HD13	1.64	0.62
1:A:96:ILE:HD11	1:A:107:HIS:HE1	1.65	0.61
1:B:254:GLN:O	1:B:258:LYS:HD3	1.99	0.61
1:C:12:LEU:HD23	1:C:19:ASN:HB3	1.80	0.61
1:B:92:LYS:HD2	1:B:130:HIS:CE1	2.36	0.61
1:C:244:GLU:OE1	1:C:244:GLU:N	2.21	0.60
1:C:105:ARG:NH2	2:C:413:HOH:O	2.33	0.60
1:A:217:LYS:NZ	2:A:410:HOH:O	2.31	0.60
1:A:100:LYS:NZ	2:A:408:HOH:O	2.26	0.60
1:A:51:PHE:CD1	1:A:56:ASN:HA	2.38	0.59
1:B:327:LEU:O	1:B:331:ILE:HG13	2.02	0.59
1:D:10:ARG:NH2	2:D:404:HOH:O	2.14	0.59
1:B:246:LYS:NZ	2:B:408:HOH:O	2.30	0.59
1:C:60:THR:HG1	1:C:67:SER:HG	1.46	0.59
1:D:240:PRO:HB2	1:D:343:TRP:CD1	2.38	0.59
1:B:166:VAL:HG23	1:B:167:LYS:HD3	1.83	0.59
1:C:67:SER:O	1:C:71:ILE:HG13	2.03	0.58
1:A:234:LYS:HE3	1:A:250:ASP:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:OH	1:A:220:LEU:HD22	2.03	0.58
1:C:78:ILE:HG13	1:C:82:TRP:HB2	1.85	0.58
1:D:92:LYS:HD2	1:D:130:HIS:CE1	2.39	0.58
1:B:70:LEU:HA	1:B:73:LYS:HG2	1.86	0.57
1:B:302:THR:O	2:B:404:HOH:O	2.17	0.57
1:D:160:GLY:HA3	1:D:189:ALA:O	2.04	0.57
1:D:241:ALA:HB1	1:D:245:LEU:HD23	1.87	0.57
1:A:145:ARG:HD3	1:A:183:ASP:OD2	2.04	0.57
1:B:84:ARG:NE	1:B:121:THR:HG21	2.19	0.57
1:A:289:LYS:O	2:A:402:HOH:O	2.16	0.57
1:A:231:ARG:HG3	1:A:265:ALA:HB2	1.86	0.57
1:B:72:GLY:HA3	1:B:118:LEU:O	2.04	0.57
1:B:234:LYS:CD	1:B:235:THR:H	2.18	0.57
1:D:20:LEU:HB2	1:D:218:LYS:HE3	1.87	0.56
1:A:6:ILE:HD12	1:A:22:PRO:HG2	1.88	0.56
1:A:232:SER:HA	1:A:253:ALA:HB1	1.85	0.56
1:B:20:LEU:HB2	1:B:218:LYS:HE3	1.86	0.56
1:B:63:TYR:OH	1:B:98:ASP:OD2	2.24	0.55
1:D:275:ARG:HG2	1:D:275:ARG:HH11	1.71	0.55
1:B:3:PHE:CD1	1:B:4:PRO:HD2	2.41	0.55
1:C:98:ASP:OD2	1:C:98:ASP:N	2.39	0.55
2:B:401:HOH:O	1:C:292:GLN:HG2	2.06	0.55
1:A:31:ASN:CG	1:A:32:ASP:H	2.10	0.55
1:A:263:GLU:O	1:A:267:PRO:HD2	2.08	0.54
1:D:96:ILE:HG22	1:D:97:THR:HG22	1.89	0.54
1:A:49:ILE:HD11	1:C:38:PRO:HB2	1.88	0.54
1:D:321:GLY:HA2	1:D:324:ASP:HB2	1.89	0.54
1:D:224:ILE:HG12	2:D:476:HOH:O	2.08	0.54
1:A:3:PHE:O	1:A:53:LYS:HE3	2.08	0.53
1:D:326:LYS:HG3	1:D:327:LEU:N	2.24	0.53
1:C:25:ILE:HG23	1:C:300:VAL:HG22	1.91	0.53
1:C:108:VAL:HG12	1:C:150:MET:HE1	1.91	0.52
1:B:241:ALA:HB1	1:B:245:LEU:HD23	1.92	0.52
1:D:96:ILE:HG22	1:D:97:THR:CG2	2.40	0.52
1:B:208:ASP:O	1:B:212:ASN:HB2	2.10	0.52
1:C:29:VAL:HG23	1:C:30:LEU:HD13	1.91	0.52
1:B:211:ILE:HG12	1:B:219:ILE:HD11	1.92	0.51
1:C:134:PHE:CD1	1:C:346:GLY:HA2	2.45	0.51
1:C:178:HIS:NE2	2:C:415:HOH:O	2.34	0.51
1:A:96:ILE:HD12	1:A:96:ILE:N	2.26	0.51
1:C:120:ASN:OD1	2:C:406:HOH:O	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:PRO:HA	1:B:287:PRO:C	2.31	0.51
1:D:229:LEU:HD21	1:D:249:VAL:HG21	1.92	0.51
1:B:232:SER:HA	1:B:253:ALA:HB1	1.92	0.51
1:B:256:LEU:HD11	1:B:327:LEU:HD11	1.93	0.51
1:B:131:ASP:OD2	2:B:405:HOH:O	2.18	0.50
1:D:263:GLU:O	1:D:267:PRO:HD2	2.11	0.50
1:A:141:TYR:O	1:A:145:ARG:HG3	2.11	0.50
1:A:228:SER:HB3	1:A:235:THR:HG22	1.94	0.50
1:A:326:LYS:HE2	2:A:401:HOH:O	2.10	0.50
1:A:137:THR:HG22	1:A:141:TYR:CE2	2.46	0.50
1:B:81:GLU:HG2	1:B:82:TRP:CD1	2.46	0.50
1:C:91:THR:O	1:C:127:VAL:HA	2.11	0.50
1:D:102:ASP:OD1	1:D:104:SER:HB3	2.11	0.50
1:D:260:SER:HB2	1:D:262:ILE:HG12	1.94	0.50
1:A:229:LEU:HD12	1:A:236:HIS:HD2	1.76	0.50
1:C:271:PHE:O	2:C:407:HOH:O	2.20	0.50
1:B:234:LYS:HD3	1:B:235:THR:OG1	2.12	0.49
1:C:25:ILE:HD11	1:C:55:LEU:HB3	1.93	0.49
1:D:245:LEU:HD12	1:D:338:HIS:HB3	1.92	0.49
1:C:96:ILE:HD11	1:C:107:HIS:NE2	2.26	0.49
1:C:108:VAL:HG12	1:C:150:MET:CE	2.42	0.49
1:D:278:PHE:CD1	1:D:288:LEU:HB3	2.47	0.49
1:C:314:ALA:O	1:C:318:GLU:HG3	2.12	0.49
1:C:63:TYR:CD2	1:C:95:ARG:HD3	2.47	0.49
1:C:266:GLU:O	1:C:270:ARG:HG3	2.12	0.49
1:C:244:GLU:H	1:C:244:GLU:CD	2.14	0.49
1:C:25:ILE:CD1	1:C:55:LEU:HB3	2.43	0.49
1:D:2:ASN:ND2	2:D:424:HOH:O	2.45	0.49
1:B:234:LYS:NZ	2:B:425:HOH:O	2.45	0.48
1:A:20:LEU:HB2	1:A:218:LYS:HE3	1.95	0.48
1:C:250:ASP:O	1:C:254:GLN:HG2	2.13	0.48
1:B:44:GLN:O	1:B:48:SER:OG	2.28	0.48
1:B:244:GLU:O	1:B:248:LYS:N	2.44	0.48
1:B:225:LEU:HD23	1:B:231:ARG:HG2	1.95	0.48
1:B:325:GLU:O	1:B:329:GLU:HG2	2.14	0.48
1:D:269:THR:O	1:D:273:MET:HG3	2.13	0.48
1:B:264:LEU:O	1:B:267:PRO:HD2	2.13	0.48
1:C:103:TYR:OH	1:C:130:HIS:O	2.30	0.48
1:A:31:ASN:CG	1:A:32:ASP:N	2.68	0.47
1:A:283:GLN:CD	2:A:402:HOH:O	2.51	0.47
1:A:288:LEU:HB3	2:A:402:HOH:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:CYS:HB3	1:B:185:GLY:O	2.14	0.47
1:A:315:ASP:HA	1:A:319:LYS:HD3	1.97	0.47
1:A:15:TYR:O	1:D:148:ARG:NH2	2.47	0.47
1:B:146:GLU:O	1:B:150:MET:HG3	2.14	0.47
1:B:315:ASP:O	1:B:319:LYS:HB2	2.14	0.47
1:D:6:ILE:HD12	1:D:22:PRO:HG2	1.97	0.47
1:D:78:ILE:HD13	1:D:82:TRP:HB2	1.97	0.47
1:A:215:GLY:O	1:D:186:ARG:NH2	2.47	0.47
1:B:308:SER:O	1:B:311:LYS:HB3	2.14	0.47
1:A:148:ARG:NH1	1:A:152:GLU:OE1	2.48	0.47
1:B:205:GLU:OE2	2:B:407:HOH:O	2.21	0.47
1:A:226:SER:O	1:A:239:HIS:NE2	2.47	0.46
1:B:29:VAL:HG21	1:B:300:VAL:O	2.16	0.46
1:C:87:TYR:HE2	1:C:89:ILE:HD11	1.80	0.46
1:C:311:LYS:NZ	1:C:315:ASP:OD2	2.45	0.46
1:B:16:SER:OG	1:B:18:VAL:HG22	2.15	0.46
1:D:137:THR:HG22	1:D:141:TYR:CE2	2.51	0.46
1:B:302:THR:N	2:B:404:HOH:O	2.44	0.46
1:B:96:ILE:HD12	1:B:100:LYS:O	2.15	0.46
1:D:37:ASP:HB3	1:D:40:LYS:HD2	1.98	0.46
1:A:53:LYS:HG3	1:A:310:LEU:HD11	1.97	0.46
1:A:72:GLY:HA3	1:A:118:LEU:O	2.16	0.46
1:D:220:LEU:HG	1:D:295:SER:HB2	1.98	0.46
1:B:270:ARG:NH2	1:B:324:ASP:OD2	2.43	0.46
1:D:66:ARG:NH1	2:D:428:HOH:O	2.49	0.46
1:C:330:GLU:O	1:C:334:LYS:HG3	2.17	0.45
1:C:92:LYS:HD2	1:C:130:HIS:CE1	2.52	0.45
1:B:33:ILE:O	1:B:34:TYR:HB2	2.16	0.45
1:C:101:PHE:CZ	1:C:134:PHE:CD2	3.04	0.45
1:C:315:ASP:HA	1:C:319:LYS:HG3	1.98	0.45
1:D:217:LYS:HG3	2:D:475:HOH:O	2.16	0.45
1:D:321:GLY:CA	1:D:324:ASP:HB2	2.47	0.45
1:B:300:VAL:HB	2:B:404:HOH:O	2.15	0.45
1:A:39:THR:HB	1:C:303:VAL:HG11	1.98	0.45
1:B:70:LEU:HD22	1:B:73:LYS:HD3	1.98	0.45
1:B:84:ARG:HE	1:B:121:THR:HG21	1.81	0.45
1:A:37:ASP:HB3	1:A:40:LYS:CG	2.45	0.45
1:A:53:LYS:HD3	1:A:53:LYS:HA	1.76	0.45
1:C:134:PHE:CE1	1:C:346:GLY:HA2	2.52	0.45
1:B:226:SER:O	1:B:239:HIS:NE2	2.45	0.45
1:C:264:LEU:HD12	1:C:264:LEU:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:HB3	2:A:428:HOH:O	2.17	0.44
1:A:207:TYR:CZ	1:A:211:ILE:HG13	2.53	0.44
1:B:31:ASN:ND2	1:B:33:ILE:HD13	2.31	0.44
1:C:145:ARG:NE	1:C:183:ASP:OD2	2.44	0.44
1:D:326:LYS:HG3	1:D:327:LEU:H	1.83	0.44
1:C:32:ASP:HB3	1:C:66:ARG:CZ	2.48	0.44
1:D:60:THR:O	1:D:91:THR:HA	2.18	0.44
1:D:96:ILE:O	2:D:406:HOH:O	2.21	0.44
1:C:9:THR:O	1:C:86:ARG:NH2	2.51	0.44
1:C:124:LEU:O	1:C:156:ILE:HA	2.18	0.44
1:B:73:LYS:HG3	1:B:74:ALA:N	2.33	0.44
1:B:168:LEU:HB2	1:B:348:TYR:CD2	2.53	0.44
1:A:189:ALA:HA	1:A:218:LYS:O	2.18	0.44
1:C:270:ARG:HG2	1:C:312:SER:HB3	2.00	0.44
1:D:238:PHE:CD1	1:D:238:PHE:N	2.84	0.44
1:A:261:ASN:O	1:C:261:ASN:ND2	2.51	0.43
1:B:11:VAL:HG12	1:B:85:GLU:O	2.18	0.43
1:A:175:LYS:HG2	1:A:180:TYR:CE2	2.53	0.43
1:B:186:ARG:NH2	1:C:215:GLY:O	2.52	0.43
1:C:245:LEU:HD13	1:C:338:HIS:HB3	2.01	0.43
1:B:97:THR:OG1	1:B:98:ASP:N	2.51	0.43
1:B:183:ASP:OD1	1:B:183:ASP:N	2.42	0.43
1:D:78:ILE:CD1	1:D:82:TRP:HB2	2.48	0.43
1:A:109:ARG:HG2	1:A:113:LYS:HD2	2.01	0.43
1:C:33:ILE:O	1:C:36:GLU:HG2	2.18	0.43
1:C:12:LEU:H	1:C:12:LEU:CD2	2.32	0.43
1:C:189:ALA:HA	1:C:218:LYS:O	2.19	0.43
1:C:327:LEU:O	1:C:331:ILE:HG13	2.18	0.43
1:D:284:LYS:HB3	1:D:285:ASP:H	1.56	0.43
1:D:270:ARG:HG2	1:D:316:VAL:HG23	2.00	0.42
1:B:235:THR:HG22	1:B:236:HIS:H	1.84	0.42
1:C:101:PHE:CZ	1:C:134:PHE:HD2	2.37	0.42
1:D:141:TYR:CE1	1:D:172:ILE:HG23	2.54	0.42
1:B:332:ILE:HG12	1:B:339:PHE:CE1	2.54	0.42
1:C:4:PRO:HA	1:C:5:PRO:HD3	1.96	0.42
1:A:52:SER:HB3	1:A:82:TRP:HZ2	1.84	0.42
1:A:259:THR:HG22	1:A:260:SER:OG	2.19	0.42
1:A:245:LEU:HD13	1:A:338:HIS:HB3	2.00	0.42
1:B:2:ASN:HB3	1:B:3:PHE:H	1.58	0.42
1:D:91:THR:O	1:D:127:VAL:HA	2.20	0.42
1:D:242:SER:O	1:D:246:LYS:HG3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:O	1:A:254:GLN:HG2	2.20	0.42
1:B:96:ILE:HG23	2:B:499:HOH:O	2.19	0.42
1:D:320:ASP:HA	2:D:403:HOH:O	2.18	0.42
1:B:33:ILE:HD11	1:B:34:TYR:CE2	2.54	0.42
1:C:84:ARG:HA	1:C:87:TYR:CZ	2.55	0.42
1:A:137:THR:O	1:A:140:VAL:N	2.45	0.42
1:D:30:LEU:HD21	1:D:41:LEU:HD22	2.02	0.41
1:C:105:ARG:HD2	1:C:146:GLU:OE1	2.20	0.41
1:B:135:VAL:HG12	1:B:139:GLU:HB2	2.01	0.41
1:D:66:ARG:HH12	1:D:69:GLU:HG2	1.84	0.41
1:D:199:GLN:HB3	2:D:501:HOH:O	2.20	0.41
1:D:66:ARG:HH11	1:D:66:ARG:HB3	1.86	0.41
1:B:128:TYR:HA	1:B:160:GLY:O	2.21	0.41
1:B:301:SER:N	2:B:404:HOH:O	2.53	0.41
1:D:66:ARG:HH12	1:D:69:GLU:CG	2.34	0.41
1:C:105:ARG:HD3	1:C:146:GLU:HB2	2.02	0.41
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.81	0.41
1:C:325:GLU:O	1:C:329:GLU:HG3	2.21	0.41
1:D:33:ILE:H	1:D:33:ILE:HG12	1.69	0.41
1:D:140:VAL:HG11	1:D:172:ILE:HD13	2.03	0.41
1:D:246:LYS:HB2	1:D:246:LYS:HE3	1.76	0.41
1:A:226:SER:HB3	1:A:229:LEU:HB3	2.03	0.41
1:C:109:ARG:HA	1:C:150:MET:CE	2.50	0.41
1:C:17:ILE:HD12	1:C:17:ILE:HA	1.87	0.40
1:C:100:LYS:HD3	1:C:100:LYS:HA	1.84	0.40
1:A:236:HIS:HB2	1:A:239:HIS:HB2	2.03	0.40
1:B:17:ILE:HD12	1:B:17:ILE:HA	1.92	0.40
1:B:51:PHE:CD1	1:B:56:ASN:HA	2.56	0.40
1:B:331:ILE:O	1:B:335:LEU:HG	2.21	0.40
1:D:124:LEU:O	1:D:156:ILE:HA	2.20	0.40
1:D:167:LYS:HE3	1:D:167:LYS:HB3	1.94	0.40
1:B:73:LYS:HG3	1:B:74:ALA:H	1.86	0.40
1:B:90:CYS:HA	1:B:126:LEU:O	2.21	0.40
1:B:266:GLU:HG2	1:B:267:PRO:N	2.37	0.40
1:C:13:GLN:HA	1:C:14:PRO:C	2.41	0.40
1:C:274:LYS:HB2	1:C:316:VAL:HG13	2.04	0.40
1:C:300:VAL:HG23	1:C:300:VAL:O	2.21	0.40
1:D:231:ARG:HA	2:D:473:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:THR:OG1	1:D:32:ASP:OD2[1_655]	1.99	0.21

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	345/351 (98%)	327 (95%)	17 (5%)	1 (0%)	41	30
1	B	346/351 (99%)	322 (93%)	21 (6%)	3 (1%)	17	8
1	C	344/351 (98%)	325 (94%)	18 (5%)	1 (0%)	41	30
1	D	339/351 (97%)	316 (93%)	18 (5%)	5 (2%)	10	3
All	All	1374/1404 (98%)	1290 (94%)	74 (5%)	10 (1%)	22	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	LYS
1	A	237	ALA
1	B	233	GLY
1	C	336	GLY
1	D	33	ILE
1	D	35	THR
1	B	234	LYS
1	D	34	TYR
1	D	3	PHE
1	D	37	ASP

5.3.2 Protein sidechains [i](#)

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	305/308 (99%)	293 (96%)	12 (4%)	32	19
1	B	306/308 (99%)	292 (95%)	14 (5%)	27	14
1	C	304/308 (99%)	287 (94%)	17 (6%)	21	9
1	D	303/308 (98%)	287 (95%)	16 (5%)	22	10
All	All	1218/1232 (99%)	1159 (95%)	59 (5%)	25	12

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	A	81	GLU
1	A	100	LYS
1	A	122	ASP
1	A	186	ARG
1	A	217	LYS
1	A	226	SER
1	A	285	ASP
1	A	311	LYS
1	A	326	LYS
1	A	333	LYS
1	A	349	SER
1	B	2	ASN
1	B	33	ILE
1	B	142	ASP
1	B	157	LYS
1	B	228	SER
1	B	229	LEU
1	B	231	ARG
1	B	236	HIS
1	B	258	LYS
1	B	260	SER
1	B	284	LYS
1	B	289	LYS
1	B	312	SER
1	B	320	ASP
1	C	32	ASP
1	C	35	THR
1	C	99	THR
1	C	110	GLU
1	C	137	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	142	ASP
1	C	155	LEU
1	C	183	ASP
1	C	226	SER
1	C	228	SER
1	C	234	LYS
1	C	281	GLN
1	C	284	LYS
1	C	285	ASP
1	C	298	LEU
1	C	303	VAL
1	C	349	SER
1	D	2	ASN
1	D	10	ARG
1	D	32	ASP
1	D	66	ARG
1	D	85	GLU
1	D	97	THR
1	D	104	SER
1	D	142	ASP
1	D	205	GLU
1	D	255	ASP
1	D	285	ASP
1	D	301	SER
1	D	323	GLU
1	D	324	ASP
1	D	326	LYS
1	D	349	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	B	236	HIS
1	C	13	GLN
1	C	281	GLN
1	C	338	HIS

5.3.3 RNA

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](#)

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	347/351 (98%)	0.67	22 (6%) 20 28	22, 34, 50, 62	0
1	B	348/351 (99%)	0.81	31 (8%) 9 15	24, 41, 59, 71	0
1	C	346/351 (98%)	0.60	17 (4%) 29 39	21, 37, 54, 60	0
1	D	343/351 (97%)	0.67	18 (5%) 27 37	24, 40, 57, 76	0
All	All	1384/1404 (98%)	0.69	88 (6%) 19 28	21, 38, 56, 76	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	ALA	6.6
1	B	1	MET	6.0
1	D	238	PHE	5.2
1	B	232	SER	4.8
1	A	349	SER	4.4
1	C	348	TYR	4.2
1	A	237	ALA	4.1
1	B	43	ILE	4.1
1	D	3	PHE	4.1
1	A	232	SER	4.0
1	B	257	LYS	4.0
1	A	233	GLY	4.0
1	C	20	LEU	3.8
1	A	3	PHE	3.7
1	D	256	LEU	3.5
1	B	259	THR	3.4
1	A	220	LEU	3.3
1	C	220	LEU	3.3
1	D	220	LEU	3.2
1	D	297	VAL	3.2
1	A	24	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	18	VAL	3.2
1	B	234	LYS	3.1
1	A	219	ILE	3.1
1	B	247	ALA	3.0
1	B	319	LYS	3.0
1	C	17	ILE	3.0
1	A	348	TYR	2.9
1	C	36	GLU	2.9
1	D	252	VAL	2.8
1	A	4	PRO	2.7
1	A	296	ILE	2.7
1	B	233	GLY	2.7
1	D	20	LEU	2.7
1	B	237	ALA	2.6
1	A	297	VAL	2.6
1	A	126	LEU	2.6
1	D	4	PRO	2.6
1	A	190	ILE	2.6
1	B	6	ILE	2.6
1	B	297	VAL	2.6
1	B	238	PHE	2.5
1	B	220	LEU	2.5
1	C	259	THR	2.5
1	B	262	ILE	2.5
1	B	260	SER	2.5
1	B	3	PHE	2.5
1	D	331	ILE	2.5
1	A	191	LEU	2.5
1	C	232	SER	2.4
1	A	327	LEU	2.4
1	D	1	MET	2.4
1	B	126	LEU	2.4
1	D	230	LEU	2.4
1	A	17	ILE	2.4
1	A	96	ILE	2.4
1	D	299	GLY	2.4
1	B	322	ALA	2.4
1	B	191	LEU	2.3
1	C	216	ILE	2.3
1	C	160	GLY	2.3
1	B	243	VAL	2.3
1	B	189	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	103	TYR	2.3
1	B	34	TYR	2.3
1	B	348	TYR	2.3
1	B	32	ASP	2.3
1	C	6	ILE	2.3
1	C	126	LEU	2.3
1	B	261	ASN	2.2
1	D	2	ASN	2.2
1	A	203	LEU	2.2
1	C	256	LEU	2.2
1	C	76	LYS	2.2
1	C	98	ASP	2.2
1	B	282	PRO	2.2
1	C	189	ALA	2.2
1	D	295	SER	2.2
1	B	80	ALA	2.2
1	B	236	HIS	2.1
1	C	187	VAL	2.1
1	D	17	ILE	2.1
1	D	191	LEU	2.1
1	D	255	ASP	2.1
1	A	254	GLN	2.1
1	D	254	GLN	2.1
1	A	204	PHE	2.0
1	B	57	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.